# 20th General Conference
# Condesed Matter Division
# EPS



# Prague, July 19-23, 2004



# BOOK OF ABSTRACTS

20th General Conference of the

# CONDENSED MATTER DIVISION

of the European Physical Society

Prague, Czech Republic, 19–23 July, 2004

## Content

## Auspices:

Prof. Ivan Wilhelm, the Rector of the Charles University in Prague
Prof. Helena Ilnerová, the President of Academy of Sciences of the Czech Republic
MUDr. Pavel Bém, the Mayor of Prague

# Conference Committees

## Organizing Committee

| | |
|---|---|
| Conference Chair: | V.Sechovský (Charles University, Prague) |
| Conference Co-Chair: | M.Glogarová (Academy of Sciences, Prague) |
| Programme: | B.Velický (Charles University, Prague) |
| Secretary: | F. Chmelík (Charles University, Prague) |
| Treasurer: | J.Šebek (Academy of Sciences, Prague) |
| Sponsorship & Exhibition: | E.Hulicius, T.Šimeček (Academy of Sciences, Prague) |
| | K.Mikšová (Charles University, Prague) |
| Local Arrangements: | R.Kužel (Charles University, Prague) |

## International Program Committee

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P.Varga (Wien)
C.Vettier (Grenoble)
V.Vitek (Philadelphia)
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## Sponsorhip

European Union – 6. Framework Programme (Marie Curie Programme – Large Conferences)
European Physical Society (EPS)
The KITE, s.r.o. – provider of the computer technology

# Words from chairman

Ladies and Gentlemen, dear colleagues,
Welcome to Prague, welcome to CMD20

It is my privilege to cordially welcome on behalf of the organizers all of you who came to Prague, the capital of the Czech Republic, to take part in the scientific and social program of the $20^{th}$ General Conference of the Condensed Matter Division of the European Physical Society. I hope that you will enjoy not only the Conference, but also the specific atmosphere and cultural millieu of one of the oldest cities in Europe.

The General Conferences of the EPS CMD form a series with a rich and inspiring tradition. It started in Antwerp in 1980 and ever since continued in regular intervals, first every year, more recently biennially. The conferences have been entrusted to many different sites in Europe and they grew in scope, size and importance. Today, they are established as the principal meeting of the condensed matter community in Europe. The last two General conferences, in Montreux, 2000, and in Brighton, 2002 attracted over 1000 participants each. To the present meeting, more than 1000 participants have registered on the conference Web site so far. The Czech community of condensed matter physicists is proud to host the first large European conference on physics in the "new" EU countries since the Czech Republic joined the European Union in May 2004. Let me acknowledge that by this a cycle closes: Prague was previously elected as the site of the $12^{th}$ EPS CMD GC in 1992. Then, it was the first major physics conference in Eastern Europe after the Iron curtain fall in 1989.

The 5–day scientific programme starts on Monday, July 19 at 8.20 by an opening address. The Conference will close on Friday, July 23 at 12:30, at the end of the closing session. Wednesday, July 21 afternoon is free giving the participants a chance to enjoy sightseeing in Prague and surroundings. The International Program committee followed the well-tested and popular format in this conference series and composed the program of plenary talks, focused sessions with regular invited speakers and mini-colloquia with a free format suitable for discussing open questions in a wide spectrum of topics. The conference will be preceded by a tutorial Student Day and will also feature an evening session with the Nobelist A. Leggett as the speaker and a musical performance Music of the quantum.

To establish personal contacts with colleagues from all over the world, I would like to invite you to participate in the Welcome Reception that is organised at the Prague Congress Centre, the site of the Conference, on Sunday, July 18 from 18.00 to 21.00.

The conference was organized at the decision of the EPS CMD Board who asked the Czech Physical Society to do it. The Organizing Committee has been composed of colleagues predominantly from the Charles University of Prague and from the Institute of Physics of the Academy of Sciences of the Czech Republic. Scientists and students from these two institutions playing the key role in the Czech condensed matter community did most of the endless work on organizing the conference.

The Conference has been able to support participation of more than 100 young scientists from different countries by the total amount of almost 80 kEUR. This was made possible mainly owing to funds provided by European Union within the project MLCF-2003-504474 of the Marie Curie Program - Large Congresses. The EPS funding within the East-West Task Force, the IUPAP funding of women physicists coming from Eastern Europe and developing countries and support of several students provided by HMI Berlin are also acknowledged.

We wish all participants a successful and pleasant meeting.

Vladimír Sechovský
Conference Chairman

# General Information

## Scope

The conference provides a forum for presentation of research work across the full range of condensed matter physics to a wide international audience. It is a sequel to the series of the EPS-CMD conferences, which started in Antwerp, 1980. The format of the meeting will be similar to the most recent ones in the series, held in Brighton, 2002 and in Montreux, 2000, each of which attracted about 1300 participants. The conference program will include plenary talks, about 32 focused sessions with invited speakers, about 32 mini-colloquia and ample space for poster sessions. The mini-colloquia should offer space for discussing both novel and established topics, while the focused sessions will be devoted to selected important areas of condensed matter physics. The Conference will be preceded by a tutorial Student day.
The Conference language will be English.

## Conference Exhibition

The exhibition presenting publishers and providers of instrumentation, materials and techniques related to physics research and applications is organized parallel to the Conference from 19 to 22 July 2004 in the area adjacent to the Poster sessions and Refreshment area.

## Registration Desk

The registration desk will be open

at Charles University, Ke Karlovu 5, Praha 2 (within the Student Day) Sunday, July 18, 8.00 - 15.00

at Prague Conference Center
| | |
|---|---|
| Sunday, July 18 | 17.00 - 21.00 |
| Monday, July 19 | 7.30 - 17.00 |
| Tuesday, July 20 | 8.00 - 17.00 |
| Wednesday, July 21 | 8.00 - 10.00 |
| Thursday, July 22 | 8.00 - 17.00 |
| Friday, July 19 | 8.00 - 10.00 |

## Venue

All conference oral and poster sessions, as well as the exhibition and the social events will be held at the Prague Congress Center. The venue is ideally located on the city arterial road and the Metro station, only a few stops from the city center.

By Air - The Prague Ruzyne International Airport is 15 km from Prague center. There is a frequent and cheap connection by city and shuttle buses.

By Rail - The Prague main station (Praha - Hlavní/ nádraží/ is only 3 stops by the Metro, line C, from the conference site. Prague has a train connection with many European cities (Berlin, Warsaw, Budapest, Wien, Nürnberg, Hamburg etc).

By Road - Prague is easily accessible through a network of highways, motorways and first class roads connecting Prague with all important border crossings.

Prague has a very well developed network of the public city transport operating 24 hours per day at a low fare.

## Prague

Prague, the capital of the Czech Republic with more than 1 million inhabitants is an important cultural and economical center of the Central Europe. The city, more than one thousand years old, is beautifully located on the banks of the Vltava (Moldau) river and reflects many important landmarks of the European history. There are many architecture monuments, museums, theatres, concert halls, plenty of style restaurants and pubs offering delicacies of the local and international cuisine and famous Czech beers, and many other places of entertainment.

The climate of Prague is temperate. In July, the weather is usually warm and sunny, but for an occasional rain, a raincoat is recommended.

## Excursions

A wide spectrum of excursions will be offered at the AR Tour desk.

## Student Day

The Conference will be preceded by a tutorial Student day. Noted experts will give an introductory overview of selected important areas of condensed matter physics. The Student Day will be held on Sunday, July 18 in the F1 Lecture Hall of the Faculty of Mathematics and Physics of the Charles University (Ke Karlovu 5, Praha 2, right across the bridge from the Congress Center). There will be no special fee for the course.

# Program Overview

# Sunday 18 July 2004
## Student Day

| | | |
|---|---|---|
| A.Schick (Pargue) | 10:00–11:30 | Computional material science: an **ab–initio** path to properties of real material |
| L.Skrbek (Prague) | 11:30–13:00 | Macroscopic quantum physics: low temperature condensates |
| A.–P.Jauho (Lyngby) | 14:00–15:30 | Physics of small man–made structures: from mesoscopic to nanoscopic systems |
| H.R.Ott (Zürich) | 15:30–17:00 | Open problems in electron structure of condensed matter: Strong electron correlations |

# Monday 19 July 2004

## Plenary Session 8:20 – 10:00 <span style="float:right">Hall A</span>

| | | |
|---|---|---|
| 8:20 | *Conference Opening* | |
| 8:30 | D.Bimberg (Berlin) | P1A1 |
| | *Quantum Dot Nanostructures: Paradigm Changes in Semiconductor Physics* | |
| 9:15 | A.Fert (Orsay) | P1A2 |
| | *Spintronics* | |

## Focused Sessions 10:30 – 12:00

Nanoscience at large facilities <span style="float:right">Hall A</span>

| | | |
|---|---|---|
| 10:30 | S. Langridge (Rutherford Appleton Lab.) | F1A1 |
| | *Order and disorder in magnetic nanostructures as studied by polarised neutron reflectometry* | |
| 11:00 | W. Kuch (Halle) | F1A2 |
| | *Photoelectron emission microscopy of magnetic domains in layered magnetic structures* | |
| 11:30 | T.H. Metzger (Grenoble) | F1A3 |
| | *Self-organized semiconductor quantum dots in the light of synchrotron radiation* | |

Bose Einstein condensation in low- dimensional semiconductor systems <span style="float:right">Room B</span>

| | | |
|---|---|---|
| 10:30 | S. A. MacDonald (Austin) | F1B1 |
| | *Spontaneous Coherence in Bilayer Quantum Hall Systems* | |
| 11:00 | I. Spielman (Caltech) | F1B2 |
| | *Indications of excitonic superfluidy in a quantum Hall bilayer* | |
| 11:30 | P. Wachter (Zürich) | F1B3 |
| | *Evidence for a Superfluid Phase in a Solid below 20 K* | |

## Field tuned quantum criticality in 2 and 3D correlated electron systems
Room C

| | | |
|---|---|---|
| 10:30 | P. Gegenwart (Dresden) | F1C1 |
| | *Field-tuned quantum criticality in heavy fermion systems* | |
| 11:00 | A. Schofield (Birmingham) | F1C2 |
| | *Open issues in field driven quantum criticality* | |
| 11:30 | A. Mackenzie (St. Andrews) | F1C3 |
| | *Quantum criticality in 2 layer strontium ruthenate* | |

## Dynamical Mean Field Theory for real materials
Room D

| | | |
|---|---|---|
| 10:30 | D. Vollhardt (Augsburg) | F1D1 |
| | *Realistic modelling of materials with strongly correlated electrons* | |
| 11:00 | S. Biermann ( Paris) | F1D2 |
| | *Electronic structure calculations for correlated materials – some recent advances on transition metal compounds* | |
| 11:30 | A. Lichtenstein (Nijmegen) | F1D3 |
| | *Dynamical mean-field theory of half-metallic ferromagnets* | |

## Magnetic field effects in cold glasses
Room E

| | | |
|---|---|---|
| 10:30 | C. Enss (Providence) | F1E1 |
| | *Influence of nuclear spins on the low temperature properties of glasses* | |
| 11:00 | A. Wuerger (Bordeaux) | F1E2 |
| | *Dephasing of atomic tunneling by nuclear quadrupoles* | |
| 11:30 | G. Weiss (Karlsruhe) | F1E3 |
| | *Magnetic field effects of the dielectric properties of disordered solids* | |

## Manipulations at surfaces
Room F

| | | |
|---|---|---|
| 10:30 | J. Pethica (Dublin) | F1F1 |
| | *Mechanics of atomic manipulation and nano-pattern formation* | |
| 11:00 | K.-H. Rieder (Berlin) | F1F2 |
| | *Controlled manipulation of atoms and molecules on surfaces* | |
| 11:30 | R. Berndt (Kiel) | F1F3 |
| | *A fresh STS look at surface states and single impurities on metals* | |

## Topological defects in materials
Room G

| | | |
|---|---|---|
| 10:30 | M. Kleman (Paris) | F1G1 |
| | *Isometric distortions in liquid crystals with simultaneous smetic and columnar order. Helicity and frustration* | |
| 11:00 | H.-R. Trebin (Stuttgart) | F1G2 |
| | *Metadislocations in quasicrystal approximants* | |
| 11:30 | L. Lejcek (Prague) | F1G3 |
| | *Role of topological defects in liquid crystals with dipolar order* | |

## Single photon solid state sources
Room H

| | | |
|---|---|---|
| 10:30 | A.J. Shields (Cambridge) | F1H1 |
| | *Single photon devices for quantum cryptography* | |
| 11:00 | P. Michler (Stuttgart) | F1H2 |
| | *Quantum optical studies on quantum dots and on individual acceptor bound excitons in semiconductors* | |

## Electron dephasing
Hall J

| | | |
|---|---|---|
| 10:30 | Y. Imry (Weizmann Inst.) | F1J1 |

*Low-temperature dephasing of quantum interference in mesoscopic systems*

11:00    B. Altshuler (Princeton)      F1J2
*Electron dephasing: orthodox model, theory*

11:30    A. Zaikin (Karlsruhe)      F1J3
*Quantum decoherence of electrons in the ground state: persistent currents and weak localization*

## Mini–Colloquia 14:00 – 16:00

## Electronic entanglement and Bell inequalities in solid state systems
Organized by: E. Sukhorukov      Room B

A. Crepieux (Marseille)      M1B1
*Entanglement in correlated electron systems*

C. Emary (Leiden)      M1B2
*Electron-hole entanglement and teleportation*

A. V. Lebedev (Moscow)      M1B3
*Entanglement in noninteracting mesoscopic structures*

P. Samuelsson (Geneva)      M1B4
*Two-particle Aharonov-Bohm effect and entanglement in the electronic Hanbury Brown Twiss setup.*

D. Saraga (Basel)      M1B5
*Entangled electrons from Coulomb scattering in a 2DEG*

F. Taddei (Pisa)      M1B6
*Clauser-Horne inequality and entanglement in mesoscopic conductors*

## Physics of f-electron materials I. (PCFES 7)
Organized by: V. Sechovský, G.H. Lander      Room C

T. Gouder (Karlsruhe)      M1C1
*Photoemission Study at the f 5localization threshold - Pu and Am: metal, nitride and hydride*

J.-C. Griveau (Karlsruhe)      M1C2
*Actinides, Superconductivity and Mott transition : the case of Americium*

J. Singleton (Los Alamos)      M1C3
*The condensed-matter physics of Plutonium; a "heavy- fermion" element*

J. Tobin (Livermore)      M1C4
*Delocalization vs. spin-orbit splitting in the actinide 5f states*

## P-wave pairing in metals
Organized by: B. L. Gyorffy      Room D

J. F. Annett (Bristol)      M1D1
*Realistic gap models for superconducting $Sr_2RuO_4$*

M. Eschrig (Karlsruhe)      M1D2
*P-wave pairing correlations in S-F hybrid structures*

Y. Liu (Philadelphia)      M1D3
*Phase-sensitive test on odd-parity superconductivity in $Sr_2RuO_4$*

D. Manske (Stuttgart)      M1D4
*Electronic theory for normal-state spin dynamics in $Sr_2RuO_4$*

## Polyelectrolyte multilayers

Organized by: Ch. Holm, R. von Klitzing                                   Room E

R. Messina (Dusseldorf)                                                   M1E1
*Monte Carlo simulations of polylelectrolyte multilayering*

H. Möhwald (Golm)                                                         M1E2
*Smart polyelectrolyte capsules as microcontainers and reactors*

J. Rühe (Freiburg)                                                        M1E3
*Polyelectrolyte Brushes as substrates for polyelectrolyte multilayers*

G. Schneider (Strassbourg)                                               M1E4
*From functional core/shell nanoparticles to empty nanospheres*

O. Vinogradova (Mainz)                                                    M1E5
*Mechanical properties of polyelectrolyte multilayer microcapsules studied by atomic force and confocal microscopy.*

## High pressure phenomena in physics

Organized by: J. Kamarad, Z. Arnold                                       Room F

F. Rodriguez (Santander)                                                  M1F1
*High-pressure physics in material science. jahn-teller systems.*

G. Oomi (Fukuoka)                                                         M1F2
*Magnetoresistance of nanoscale magnets under high pressure*

M.I. Eremets (Mainz)                                                      M1F3
*Electric conductivity studies at megabar pressures*

A. Bergara (Bilbao)                                                       M1F4
*Group IVa hydrides at high pressure: high temperature superconductors?*

## Mechanical properties of metallic glasses

Organized by: T. Egami                                                     Room G

H. A. Davies (Sheffield)                                                   M1G1
*Bulk metallic glasses - glass formability and flow*

J. Eckert (Dresden)                                                        M1G2
*tMicrostructure design for strengthening of metallic glasses*

F. Faupel (Kiel)                                                           M1G3
*Mechanisms of diffusion and viscous flow in bulk glass- forming alloys*

A. L. Greer (Cambridge)                                                    M1G4
*Experimental observations of shear banding in bulk metallic glasses*

J. M. Pelletier (Lyon)                                                     M1G5
*Mechanical response in bulk metallic glasses: elastic, viscoelastic and viscoplastic components. Influence of a nanocrystallization.*

## Theory of optical and dielectric properties in condensed matter

Organized by: G. Onida, N. Manini                                         Room H

A. Marini (San Sebastian/Donostia)                                        M1H1
*Quasiexcitons and bound excitons in extended systems: Many–Body versus time–dependent density–functional approach*

F. Sottile (Palaiseau)                                                     M1H2
*Parameter-free calculation of response functions in time- dependent density-functional theory*

G. Vignale (Missouri)                                                      M1H3
*Time-dependent spin-current-density functional theory*

U. von Barth (Lund)                                                        M1H4
*Conserving theories for the response functions of Time- Dependent Density-Functional Theory.*

Mesoscopics
Organized by: A. P. Jauho                                    Hall J
  D. Sanchez (Geneva)                                    M1J1
  *Magnetic-field asymmetries in nonlinear mesoscopic transport*
  A. Armour (Nottingham)                                 M1J2
  *Mesoscopic mechanical systems*
  T. Novotny (Lyngby)                                    M1J3
  *Current noise in nanoelectromechanical systems*
  K. Flensberg (Copenhagen)                              M1J4
  *Electron-vibron coupling in molecular transistors*

## Poster Session 16:00–18:00

### Low dimensional systems

Michal Horak                                                 S1X1
*High Frequency Properties of Nanometer Semiconductor Structures*
H. Ness                                                      S1X2
*Coherent transport and electron-vibration coupling in molecular wires*
P. Nemec, D. Sprinzl, P. Nahalkova, F. Trojanek, P. Maly     S1X3
*Spin coherence dynamics in CdS nanocrystals at room temperature*
A. Golub                                                     S1X4
*High-order current correlation functions in the Kondo systems.*
K. Yu. Arutyunov, T. T. Hongisto                             S1X5
*NI-SQUID: Normal metal - Insulator - Superconductor Quantum Interference Device*
A. Donarini, T. Novotny, C. Flindt, A.-P. Jauho             S1X6
*Current Noise of Shuttle Devices*
A. Hospodkova, K. Kuldova, J. Oswald, E. Hulicius, J. Pangrac, I. Vavra    S1X7
*Overlaping of vertically stacked quantum dot electron wavefunctions*
Eugene Kamenetskii, Reuven Shavit, Michael Sigalov          S1X8
*Ferromagnetic magnetic-dipolar-mode quantum dots*
Eugene Kamenetskii                                           S1X9
*Anapole moments in MS-wave ferrite disks*
A. Stolovits, R. K. Kremer, Hj. Mattausch, A. Sherman, A. Simon    S1X10
*Quantum interference of electrons in $Nb_5Te_4$*
C. Flindt, T. Novotny, A. Donarini, A.-P. Jauho             S1X11
*Current noise in a vibrating quantum dot array*
Ismet I. Kaya                                                S1X12
*Directional scattering in two dimensional electron gas*
Natalia E. Kaputkina, Yuri E. Lozovik                       S1X13
*Electron and Optical Properties of Two-Dimensional and Three-Dimensional Quantum Dots in Magnetic Field*
V. N. Gladilin, V. M. Fomin, J. T. Devreese                 S1X14
*Magnetic response of superconductor nanograins*
Oktay Z. Alekperov, Niyazi M. Huseynov                      S1X15
*Polaron energy spectrum in disc shaped quantum dot*
F. Moresco, L. Gross, L. Grill, A. Gourdon, C. Joachim, K.-H. Rieder    S1X16
*Contacting a Single Molecular Wire by STM Manipulation*
Yueh-Nan Chen, Tobias Brandes, Che-Ming Li, Der-San Chuu    S1X17
*Zeno effect and shot noise spectrum of superradiant entangled excitons*

## Magnetism and strong correlations

**High pressure physics**

J. Rodriguez Fernandez, Masashi Ohashi, Atsushi Tashiro, Gendo Oomi, A. Senas, J. C. Gomez sal   S1X62
*Suppression of the martensitic transformation in TbCu and GdCu induced by pressure*
A.L. Zherebtsov, K.F. Grebyonkin, V.V. Popova   S1X63
*Modeling of intermolecular interaction potentials in dense gaseous medium based on ab initio calculations*
I. Hernandez, F. Rodriguez, H. D. Hohcheimer   S1X64
*Pressure-induced photoluminescence in $MnF_2$ at Room Temperature.*
J. Kamarad, Z. Arnold   S1X65
*Magnetic moment of Iron under high pressure*
V.Yu. Bardic, K.S. Shakun   S1X66
*Functional form of repulsive potential in high-pressure region*

## Chemical physics

N. Elsner, M. Nolte, A. Fery   S1X67
*Adhesion of Polyelectrolyte Microcapsules on Homogenous and Patterned Substrates*

## Low dimensional systems

P.S. Cornaglia, H. Ness, D.R. Grempel   S1Y101
*Many Body Effects on the Transport Properties of Single-Molecule Devices*
Karel Neudert, Frantisek Trojanek, Petr Maly   S1Y102
*Superlinear Pump Intensity Dependence of Photoluminescence in Si Nanocrystals*
A.V. Gomonnai, Yu.M. Azhniuk, M. Kranjcec, V.V. Lopushansky, I.G. Megela   S1Y103
*Optical studies of radiation effects in bulk and nanoscale $CdS_{1-x}Se_x$ semiconductors*
Juan J. Alonso, Julio F. Fernandez   S1Y104
*Magnetization relaxation of single molecule magnets at low temperatures*
J. Rammer, A. Shelankov, J. Wabnig   S1Y105
*Quantum measurement in the charge representation*
Rodica-Mariana Ion, Dragos-Viorel Brezoi   S1Y106
*Phthalocyanines Incorporated into Layered Materials*
S. N. Klimin, V. M. Fomin, F. Brosens, J. T. Devreese   S1Y107
*Optical response of many-polaron quantum dots*
O. Voskoboynikov, C.M.J. Wijers, J.J. Liu, C.P. Lee   S1Y108
*Magneto-Optical Response by a Layer of Semiconductor Nano-Rings*
R. Raimondi, G. Savona, P. Schwab, T. Lueck   S1Y109
*Electronic thermal conductivity of disordered metals*
P. S. Cornaglia, H. Ness, D. R. Grempel   S1Y110
*Many Body Effects on the Transport Properties of Single-Molecule Devices*
Pavel Jelinek, Ruben Perez, Jose Ortega, Fernando Flores   S1Y111
*First principles simulation of transport properties of metalic nanowires*
Hiroyuki Yoshimoto, Kazuo Sano, Susumu Kurihara   S1Y112
*Thermoelectric transports through charge-density-wave point contact*
Detlef Beckmann, Heiko B. Weber, Hilbert von Loehneysen   S1Y113
*Nonlocal transport in superconductor-ferromagnet hybrid structures*

**Material Science**

**Chemical physics**

**Theory**

V. Drchal, J. Kudrnovsky, S. Khmelevskyi, B.L. Gyorffy, P. Mohn, P. Weinberger   S1Z222
*Exchange interactions in spin glass alloys*
J. Houserova, M. Sob   S1Z223
*Ab initio study of C14 Fe-Mo Laves compounds*
L. M. Ghiringhelli, J. H. Los, E. J. Meijer, A. Fasolino, D. Frenkel   S1Z224
*High pressure diamond-like liquid carbon*
T. Schmidt, H. Solbrig   S1Z225
*The influence of local coordination polyhedra on bonding properties in Al- TM(transition metal) alloys*
P. Bokes, R. Godby   S1Z226
*Conductance, polarisation and strength of Drude singularity in quantum junctions*
M. G. Shelyapina, V. S. Kasperovich, D. Fruchart, N. Skryabina, E. K. Hlil, P.   S1Z227
*Ground properties of transition metal disordered alloys: a KKR-CPA study*
Kurt Scheerschmidt, Volker Kuhlmann, Alexandre Yu Belov   S1Z228
*Relaxation of interface defects: elastic boundary conditions and bond order potentials in empirical molecular dynamics simulations*

# Tuesday 20 July 2004

## Plenary Session 8:30 – 10:00 <span style="float:right">Hall A</span>

8:30    D. Pettifor (Oxford)   P2A1
        it Bond-order potentials : bridging the electronic to atomistic modeling hierarchies
9:15    M. Roukes (Caltech)   P2A2
        *Nanomechanical Systems*

## Focused Sessions 10:30 – 12:00

New frontiers in Bose-Einstein Condensation <span style="float:right">Room B</span>
10:30   G. Baym (Urbana)   F2B1
        *The physics of rapidly rotating Bose-Einstein condensates*
11:00   M. Machholm (Copenhagen)   F2B2
        *Spatial period-doubling in Bose-Einstein condensates in an optical lattice*
11:30   B. Paredes (Garching)   F2B3
        *Tonks gas of ultracold atoms in an optical lattice*

Ferromagnetic semiconductor materials and spintronic devices <span style="float:right">Room C</span>
10:30   J. Sinova (Texas A&M University)   F2C1
        *Magneto-optic effects and magnetization dynamics in metallic ferromagnetic semi-conductors*
11:00   B. Gallagher (Nottingham)   F2C2
        *GaMnAs materials development, magneto-transport and spintronics*
11:30   L. Molenkamp (Wurzburg)   F2C3
        *Spintronic nanostructures*

## Plutonium-based Superconductivity
Room D

| 10:30 | F. Wastin (Karlsruhe) | F2D1 |

*Magnetic and superconducting behavior in PuRhGa5 and related compounds*

| 11:00 | J. Sarrao (Los Alamos) | F2D2 |

*Tuning unconventional superconductivity in CeMIn5 and PuMGa5*

| 11:30 | P. Oppeneer (Dresden) | F2D3 |

*Electronic structure of the Pu-based superconductors PuCoGa5 and PuRhGa5*

## Soft condensed matter at large facilities
Room E

| 10:30 | G. Fragneto (Grenoble) | F2E1 |

*Fluctuations of model membranes: complementarity of neutron and X-ray studies*

| 11:00 | L. Leiserowitz (Weizmann Inst.) | F2E2 |

*Crystalline thin film architectures at the air-liquid interface*

| 11:30 | C. Riekel (Grenoble) | F2E3 |

*On possibilities of micro X-ray diffraction for soft condensed matter*

## Epitaxial organic thin films
Room F

| 10:30 | F. Meyer zu Heringdorf (Essen) | F2F1 |

*Growth dynamics of pentacene thin films*

| 11:00 | B. Krause (Grenoble) | F2F2 |

*PTCDA on Ag - a model system for organic epitaxy*

| 11:30 | S.R. Forrest (Princeton) | F2F3 |

*The role of triplet excitons in organic electronic devices*

## Physics of the cascade lasers
Room G

| 10:30 | R. Teissier (Montpellier) | F2G1 |

*Antimonide quantum cascade lasers*

| 11:00 | A. Wacker (Lund) | F2G2 |

*Modelling of quantum cascade lasers*

## From femto towards attosecond time scale in solids
Room H

| 10:30 | M. Wegener (Karlsruhe) | F2H1 |

*Extreme nonlinear optics with few-cycle pulses in semiconductors*

| 11:00 | G. Reider (Wien) | F2H2 |

*Time resolved attosecond spectroscopy: looking into atoms*

| 11:30 | D. von der Linde (Essen) | F2H3 |

*Ultrafast X-ray diffraction*

## Physics of nanomaterials
Hall J

| 10:30 | G. Bauer (Linz) | F2J1 |

*Growth and structural properties of low-dimensional nanostructures*

| 11:00 | R. Woodward (University of West.Australia) | F2J2 |

*Nanosecond dynamics of magnetic films and nanostructures*

| 11:30 | J. Cizek (Prague) | F2J3 |

*Investigation of defects in ultra fine grained metals by positron annihilation spectroscopy*

## Mini–Colloquia 14:00 – 16:00

Turbulence in coherent quantum systems and connections to general hydro-dynamics

Organized by: L. Skrbek, C. F. Barenghi                                    Room B

  K.R. Sreenivasan (Trieste)                                            M2B1
  *Classical and quantum turbulence*
  M. Tsubota (Osaka)                                                    M2B2
  *Numerical simulation on quantum turbulence*
  P. McClintock (Lancaster)                                             M2B3
  *Creation and decay of quantum turbulence in He II*
  M. Krusius (Helsinki)                                                 M2B4
  *Turbulence in rotating superfluid 3He-B*

Physics of f-electron materials II. (PCFES 7) Organized by: V. Sechovský, G.H.
Lander                                                                      Room C
  E. Blackburn (Grenoble)                                               M2C1
  *The magnetic response of an antiferromagnetic superconductor, UPd2Al3*
  R. Caciuffo (Ancona)                                                  M2C2
  *Polarisation of spin waves in UO2*
  K. Prokes (Berlin)                                                    M2C3
  *Stability of AF structure in UNiAl in magnetic fields*
  R. Walstedt (Tokai)                                                   M2C4
  *Ligand NMR studies of neptunium compounds*

Quantum criticality in heavy-fermion metals and ruthenates

Organized by: F. Steglich, P. Coleman                                       Room D
  S. Grigera (St. Andrews)                                              M2D1
  *Metamagnetism and quantum fluctuations in the ruthenate Sr3Ru2O7*
  S. Bü hler-Paschen (Dresden)                                          M2D2
  *Hall effect at a heavy-fermion quantum critical point*
  A. Schröder (Kent)                                                    M2D3
  *Magnetic fluctuations close to an antiferromagnetic quantum critical point as observed in Ce(Cu,Au)6 and CeNi2Ge2*

## New generation of intermetallics
Organized by: V. K. Pecharsky, E. Brück                                      Room E
K. H. J. Buschow (Amsterdam)                                                 M2E1
*Magnetocaloric properties of Fe(Mn) based intermetallics for room temperature magnetic refrigeration*
A. Fujita (Sendai)                                                           M2E2
*Application of the itinerant-electron metamagnetic transition in La(FexSi1 - x)13 compounds to high- performance magnetic refrigerants by hydrogen absorption*
S. Gama (Campinas)                                                           M2E3
*Comparison of MnAs and GdGeSi intermetallics under pressure in terms of the colossal magnetocaloric effect*
K.A. Gschneidner (Ames Laboratory)                                           M2E4
*The magnetocaloric effect in intermetallic compounds and their role in magnetic refrigeration*
L. Morellon (Zaragoza)                                                       M2E5
*Interplay of structure and magnetism in R5(SixGe1-x)4*
H. Yamada (Matsumoto)                                                        M2E6
*Strong magnetocaloric effect in transition-metal compounds*

## Physics in high magnetic fields
Organized by: F. Pobell                                                       Room F
J. Haase (Dresden)                                                           M2F1
*Nuclear Magnetic Resonance in High Pulsed Magnetic Fields*
M. Jaime (Los Alamos)                                                        M2F2
*Localized, Itinerant, and Superfluid Spin Triplons in Quantum Magnets*
J.K. Maan (Nijmegen)                                                         M2F3
*Suppression of interlayer coupling in semiconductor bi-layers in high magnetic fields*
J. Mydosh (Leiden)                                                           M2F4
*Why we need high magnetic fields in strongly correlated electron physics: the case of URu2Si2*
Ch. Rüegg (Zürich)                                                           M2F5
*Bose-Einstein condensation of the triplet states in the magnetic insulator TlCuCl3*

## Multiscale modelling
Organized by: Ch. Elsaesser                                                   Room G
J.-L. Martin (Lausanne)                                                      M2G1
*Novel aspects of the dislocation mechanisms in DC covalent crystals.*
M. Moseler (Freiburg)                                                        M2G2
*Bridging the length scales by hybrid molecular dynamics*
M. Mrovec (Karlsruhe)                                                        M2G3
*From an ideal crystal to a microstructure: Multiscale modeling of bcc transition metals*
V. Paidar (Prague)                                                           M2G4
*Mixing and separation in binary alloys of transition metals*
P. Schiffels (Bremen)                                                        M2G5
*Towards a multiscale modelling of adhesive joints: extending atomistic simulations to the interphase*
M. Sob (Brno)                                                                M2G6
*Theoretical strength and high-strain elasticity of intermetallic compounds from first principles*

## Boron-based III-V compound semiconductors
Organized by: K. Terashima, T. Udagawa                                    Room H
H. Dumont (Lyon)                                                          M2H1
*Photoluminescence and structural investigation of BGaAs/GaAs epilayers*
Y. Kumashiro (Yokohaka)                                                   M2H2
*Preparations and semiconducting properties of boron phosphide and boron antimonide*
H. Nakanishi (Toshiba)                                                    M2H3
*Epitaxial growth 3C-SiC on Si(100) substrate using a BP buffer layer*
T. Udagawa (Saitama)                                                      M2H4
*Structural investigation of hetero-interface of transparent (111)-BP layer and (111)-GaP substrate*
K. Watanabe (Tsukuba)                                                     M2H5
*Direct-bandgap properties of hexagonal boron nitride*
A. Zaoui (Aachen)                                                         M2H6
*Bonds and bands in boron compounds*

## Quantum dots for quantum computing
Organized by: D. Vvedensky                                                Hall J
M. Atature (Zürich)                                                       M2J1
*All-optical detection of electron spin in a single quantum dot*
C. Barnes (Cambridge)                                                     M2J2
*Quantum computation using electrons trapped by surface acoustic waves*
E. Kapon (Lausanne)                                                       M2J3
*Site- and energy-controlled semiconductor quantum dots for quantum information processing applications*

## Poster Session 16:00–18:00

**Magnetism and strong correlations**

A.V. Andreev, A.V. Kolomiets, S. Danis, T. Goto                          S2X1
*Magnetoelasticity of $R_2 T_{13.6} Si_{3.4}$ ( $R = U, Lu; T = Fe, Co$ )*
Martin Divis, Jan Rusz, Vladimir Nekvasil                                S2X2
*LDA+U calculation of the crystal field interaction in $PrO_2$*
A. Vlcek, M. Orendac, A. Orendacova, T. Fennel, S. T. Bramwell           S2X3
*Experimental study of magnetocaloric effect in dipolar spin ice $Dy_2Ti_2O_7$*
L.P. Ferreira, M.D.Carvalho, M.M. Cruz, M. Godinho                       S2X4
*Transport and Magnetic Properties of $(Sr,A)RuO_3$ ( $A = K, Na$ )*
Ilja Turek, Jan Rusz, Martin Divis                                       S2X5
*Origin of the negative volume magnetostriction of $GdAl_2$ compound*
F. C Tsao, T. -N Li, P. J Hwung, M. K Chung, C. C Yang, K. -H Lii, W. -H Li   S2X6
*Intra and inter layer magnetic coupling of V in Cu0.5(VOAsO4)*
M.S. Vasconcelos, E.S. Guimaraes, E.L. Albuquerque                       S2X7
*Spin Canted Polaritons in Ultra-Thin Antiferromagnet Films*
Daniela Todoran, Marin Coldea, Radu Todoran                              S2X8
*X-ray photoelectron spectroscopy and magnetism of the $Al_4GdNi$ AND $Al_6GdNi_3$ compounds*
T. Kana, D. Legut, M. Sob                                                S2X9
*Searching for magnetism in palladium in face-centered and body-centered cubic crystal structure*

M. Sikora, D. Zajac, C.J. Oates, M. Borowiec, D. Rybicki, Cz. Kapusta, D. Serrate, J.M. De Teresa, M.R. Ibarra S2X10
*XMCD study of double perovskites (Sr,Ba,Ca)2FeReO6*
S.S. Sosin, L.A. Prozorova, A.I. Smirnov, O.A. Petrenko, M.E. Zhitomirsky S2X11
*Magnetocaloric effect in a pyrochlore magnets $Gd_2Ti_2O_7$*
K. Tibenska, A. Vlcek, T. Papageorgiou, J. Chomic, M. Orendac, A. Orendacova, A.Feher
S2X12
*Magnetic properties of $Cu(NH_3)_2Ag(CN)_4$ - A quasi 2D heisenberg antiferromagnet*
E. Cizmar, M. Kajnakova, M. Orendac, A. Orendacova, A. Feher, J.-H. Park, M.W.Meisel
S2X13
*Experimental study of two-dimensional square-lattice magnets*
S. Abe, D. Takahashi, J. Yoshida, H. Shinjo, K. Matsumoto, H. Suzuki, T. Kitai S2X14
*Nuclear Magnetism of $PrPb_3$ in the Antiferro-quadrupolar Ordered state.*
Yu.A. Shakhayeva, D.N.Merenkov, A.B. Chizhik, S.L. Gnatchenko, M. Baran, R.Szymczak, V.O. Vas'kovskiy, A.V. Svalov S2X15
*Coercivity properties of Gd/Si/Co multilayers with ferrimagnetic ordering*
A.A. Ostroukhova, F.O. Schumann, R. Thamankar S2X16
*Dependence of magnetic properties from thickness and content of material in ultrathin films.*
Takao Mori S2X17
*A One-Dimensional Magnetic System; Terbium Borosilicide*
K.Miliyanchuk, L. Havela, A.V. Kolomiets, A.V. Andreev S2X18
*Hydrogen–induced variations of UTSn magnetism*
H. Michor, E. Bauer, G. Hilscher, C. Hofstaetter, R. Lackner, M. Sieberer, A. Gribanov, Yu. Seropegin, P. Rogl S2X19
*Magnetic properties of $REPt_3Si$*
N.M. Ferreira, S.K. Mendirata, M.A. Valente, M.A. Sa, J.M. Brochado Oliveira, J.M.Machado da Silva S2X20
*Precipitation of Magnetic Oxide in $_xFe_2O_3$ (1-x) [MO $2B_2O_3$] Glasses; The Effect of Magnetic Field during Precipitation*
M. Zentkova, M.Mihalik, J. Kamarad, M Baanda, Z. Arnold, R. Podgajny, B. S2X21
*High pressure effect on ferromagnetic ordering in layered copper*
Pavel Svoboda, Jana Vejpravova, Mathias Doerr, Michael Loewenhaupt, Martin Rotter
S2X22
*Magnetocaloric effect on $TbCu_2$ single crystal*
O. Kravchyna, A. Kaplienko, A. Anders, M. Kajnakova, A. Feher S2X24
*EPR spectra of powder sample $Cu(imid)_4SO_4$*
Andrew P. Sazonov, I.O. Troyanchuk, D.M. Tobbens S2X25
*Two magnetic phases in $LaCo_{0.5}Mn_{0.5}O_3$ perovskite*
A. Orendacova, A. Vlcek, M. Orendac, O. V. Kravchyna, M. Kajnakova, J. Cernak, A. G. Anders, A. Feher S2X26
*ESR studies of a quasi-tetrameric compound*
$[Cu^{II}(en)_2(H_2O)][Cu^{II}(en)_2Ni_2Cu_2^I(CN)_{10}]\cdot 2H_2O$
H. Yamada S2X27
*Magnetic states of $MgCo_2$ and $CaCo_2$ with Laves phase structures*
F. Firpo, A.Ubaldini, C. Artini, M.M. Carnasciali, R. Masini, M.R. Cimberle, M.Tropeano, G.A. Costa S2X28
*Magnetic transitions in Ru - 1222 superconducting phase*
Anders Bergman, Erik Holmstrom, Olle Eriksson S2X29
*Magnetism of Fe clusters embedded in Co*

## Materials science

N. Tareuchi, M. Hiroi, K. Gosho, M. Kawakami                                    S2Y101
*Structural, Electrical Transport, and Magnetic Properties of a half-Heusler Compound Co-TiSb*
N.I. Klyui, V.G. Litovchenko, A.N. Lukyanov                                       S2Y102
*Effective antireflecting diamond-like carbon coatings for Si-solar cells*
S. Yoon, S. H. Phark, Z. G.Khim, B. J. Kim, B. J. Suh, J. Kim                     S2Y103
*SPM study of $Mn_{12}O_{12}(O_2CC_4H_3S)_{16}(H_2O)_4$ molecules on Au*
E. Condrea, A. Grozav, A. Nicorici                                                 S2Y104
*ANOMALIES IN THERMOPOWER OF TENSILE-STRAINED BISMUTH NANOWIRES*
Anderson Dias, Henrique Costa Braga, Virginia S. T. Ciminelli                      S2Y105
*Microwave-hydrothermal synthesis of nanostructured magnetic ceramics from industrial effluents*
Tamar Tchelidze, Tamaz Kereselidze                                                S2Y106
*Exciton Energies and Decay Probabilities in GaN/AlN Quantum Structures*
Anderson Dias                                                                      S2Y107
*Micro-Raman spectroscopy of microwave A(B'1/3Nb2/3)O3 electroceramics*
A. Ponomarev , L. Sabirzyanova, K. Sazonova , A. Moskvin, Yu. Panov ., A. Ivanov
                                                                                   S2Y108
*Anisotropic ab - plane magnetoresistance in $Nd_{2-x}Ce_xCuO_{4+\delta}$*
Sergey V. Danik                                                                    S2Y109
*Phonon breakdown in zinc in strong magnetic fields*
Gregory Leitus, Frieda Kopnov, Alex Yoffe, Reshef Tenne                            S2Y110
*Electronic transport in compacted powder of the different shape WS2*
W.-H. Li, C. C. Yang, P. J. Hwung, F. C. Tsao, M. K. Chung                         S2Y111
*Superconducting parameters of zero-dimensional In nanoparticles*
G. Kamarchuk, A. Khotkevich, A. Zaika, P. Molinie, A. Leblanc, E. Faulques        S2Y112
*Direct determination of electron-phonon interaction in $2H\text{-}TaSe_2$*
Barbora Bartova, Dalibor Vojtech, Jan Verner, Juliana Gemperlova, Marian Cernansky
                                                                                   S2Y113
*Rapidly solidified Al-Ni-Zr alloys - microstructure and phase composition*
Valentyn Gokhfeld                                                                  S2Y114
*Non-equilibrium magnetization of electron gas in metals*
E Mulazzi, R Perego, H Aarab, L Mihut, S Lefrant, E Faulques, J Wery              S2Y115
*Optical properties of carbon NT-PPV composites : influence of the PPV conversion temperature*
Tamar Tchelidze, Tamaz Kereselidze                                                S2Y117
*Electron-Hole Coulomb Interaction in Stacks of ZnSe/CdSe Quantum Dots*
A. Osadchy, E. Obraztsova, M. Fujii, S. Hayashi, K. Imakita, K. Matsumoto         S2Y118
*Curvature influence on carbon nanotube electronic structure: modelling and photoluminescence experiments*
H. Onodera, K. Saino, A. Tobo, J. Kaya, K. Ohoyama                                S2Y119
*Field-induced Antiferroquadrupolar Order in Antiferromagnetic $Dy_{1-x}Gd_xB_2C_2(0.25\leq x\leq 0.4)$ Compounds*
O. Tegus, B. Fuquan, L. Zhang, W. Dagula, E. Bruck, F.R. de Boer, K.H.J. Bushow   S2Y120
*Magnetic-entropy change in Mn1.1Fe0.9P0.7As0.3-xGex*
Yaroslav V. Filipov, V. S. Staschuk, V. V. Vovchenko                              S2Y121
*Influence of oxide layers on copper optical properties in a wide spectral range*

Frantisek Maca, Alexander B. Shick, Peter M. Oppeneer S2Y143
*Anomalous Magnetic Anisotropy of Fe and Co Monatomic Wires at the Pt Surface Step Edge*
Mortaza Mozaffari, Jamshid Amighian, Ahmad Hasampour S2Y144
*Reduction of Calcining Temperature in Preparation of YIG Powders Using High Energy Ball Milling*
Simon Kos, Marc Achermann, Victor I. Klimov, Darryl L. Smith S2Y145
*Förster energy transfer from a quantum well to a proximal nanocrystal- quantum-dot monolayer*
K. Raftopoulos, I. Zegkinoglou, A. Vassilikou Dova, P. Pissis, A. Kanapitsas, Y. Savelyev S2Y146
*Dielectric Studies of Segmental Polyurethanes*
E. Thune, M. Seibt, P. Oelhafen, J. Howe, P. Reinke S2Y147
*Au clusters: the role of ion energy in their formation*
A.A. Velichko, A.L. Pergament, G.B. Stefanovich, N.A. Kuldin S2Y148
*Electronic switching and metal-insulator transitions in compounds of transition*
Radu Todoran, Daniela Todoran, Iulia Caraman S2Y149
*Investigation of the valence band ion the case of thin films of $RNi_5$ (R=Ce,Y,La) compounds*
Marko Budimir, Dragan Damjanovic, Nava Setter S2Y150
*Piezoelectric anisotropy - phase transition relations in perovskite single crystals*
Barbora Bartova, Dalibor Vojtech, Jan Verner, Antonin Gemperle, Vaclav Studnicka S2Y151
*Rapidly solidified Al-Cr-Fe-Si-Ti powder alloys - structure and properties*


**Soft matter**


L. A. Sanchez de Almeida Prado, C S Karthikeyan, I. Linhares de Torriani, K. Schulte, S. Pereira Nunes S2Z201
*Poly(benzimidazole)/Layered Silicate Nanocomposites: Preparation, Silicate Exfoliation and Vapor-Barrier Properties*
K. Dworecki, M. Kudzia, S. Wcasik S2Z202
*Experimental studies of anomalous diffusion in membrane-gel system*
Alexei N. Vasilev, Alexander V. Chalyi S2Z203
*Multicomponent confined system*
Emil J. Samuelsen, Dag W. Breiby, Oleg Konovalov S2Z204
*Ordering at the interface of polymeric solutions*
Carlo Cavazzoni, Renato Colle, Riccardo Farchioni, Giuseppe Grosso S2Z205
*3D - structure of Emeraldine Base polymers by Car-Parrinello molecular dynamics.*
Peter-M. Konig, Roland Roth, Klaus Mecke S2Z206
*Morphological Thermodynamics: how do free energies depend on shape?*
S. P. Kuznetsov, N. P. Saposhnikov, A. V. Shelagin, P. N. Brevnov, V. G. Grinev, N. Yu. Kovaleva, I. N. Meshkova, L. A. Novokshonova, T. M. Ushakova S2Z207
*Composites and polymer mixtures super molecular structure study by very cold neutrons scattering.*
M. S. Tomas S2Z208
*Casimir force between planar magnetodielectrics*
Atamas Nataliya, Atamas Alexander S2Z209
*Monte Carlo Study of Hydrations Effects of Polar and Non-polar Molecules in Water at (250–460)K.*
Bruno Jean, Frederic Ne, Yeshayahu Talmon, Pierre Terech S2Z210
*Self-Assembled Monodisperse Steroid Nanotubes in Water: Kinetics of Formation and Ordering*

I.P. Studenyak, O.T. Nahusko, M. Kranjcec S2Z211
*Optical and refractometric studies of $(1 - x)TiO_2 \cdot xLn_2O_3$ (Ln= Nd, Sm, Gd, Er, Yb) thin films*
Imre O. Guth, Zeljka N. Cvejic, Svetlana R.Lukic S2Z212
*The influence of iron on electronic polarizibility in glasses of Sb-S-I type*

## Low temperature physics

V. Chagovets, T. Kalko, K. Nemchenko, E. Rudavskii, G. Sheshin, A. Zadorozhko S2Z213
*Relaxation and dissipation processes in the phonon-impuriton system of superfluid mixture $^3He$ in $^4He$*
I. N. Adamenko, K. E. Nemchenko, V. A. Slipko, A. F. G. Wyatt S2Z214
*Evolution of phonon pulses in superfluid $^4He$ at different pressures*
T.V. Chagovets, M. Rotter, F. Soukup, L. Skrbek S2Z215
*Experimental Apparatus for Investigation of the Stability of the He II Flow Based on the Second Sound Attenuation Technique*
A.V. Gordeev, F. Soukup, L. Skrbek S2Z216
*Decay of Counterflow Turbulence in He II*
S. Shulga, A. Yatsenko S2Z217
*Simultaneous singlet and triplet pairing in a two- component fermi-liquid*
Maxim Yu. Brazhnikov, Viktor B. Efimov, German V. Kolmakov, Alexandr A. Levchenko, Elena V. Lebedeva, Leonid P. Mezhov-Deglin S2Z218
*Second Sound Turbulence in Superfluid Helium*
V.K. Chagovets, T.V. Kalko, E.Ya. Rudavskii, G.A. Sheshin, A.A. Zadorozhko S2Z219
*Instability of superfluid $^3He$-$^4He$ solutions under heating from below*
J. Tempere, I. F.Silvera, J. T. Devreese S2Z220
*Spherical electron systems in a multielectron bubble in liquid helium*
M. Wouters, J. Tempere, J. T. Devreese S2Z221
*Tunneling Dynamics of a Superfluid Fermi Gas*
C.F. Barenghi, D.R. Poole, Y.A. Sergeev, W.F. Vinen S2Z222
*Theory of Particle Image Velocimetry in helium II*

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19:00 – evening session

Bethlehem Chapel, the Old Town of Prague

**Nobel-Prize lecture given by A. J. Leggett**

followed by

**Performance: "Music of The Quantum"**

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# Wednesday 21 July 2004

## Plenary Session 8:30 – 9:00 <span style="float:right">Hall A</span>

8:30    M. Chan (University Park) <span style="float:right">P3A1</span>
  *Observation of the supersolid phase in solid He-4*

## Mini–Colloquia 9:15 – 11:15

### HTSC physics

Organized by: S. Maekawa <span style="float:right">Room B</span>
  W. Hanke (Wurzburg) <span style="float:right">M3B1</span>
  *Are the spin-fluctuation and the electron-phonon mediated pairing potentials enhanced or suppressed by vortex corrections?*
  B. Keimer (Stuttgart) <span style="float:right">M3B2</span>
  *Magnetic Excitations in High Temperature Superconductors*
  S. Maekawa (Sendai Japan) <span style="float:right">M3B3</span>
  *New oxide-superconductors: similarity and dissimilarity to high- temperature superconducting cuprates*
  J. M. Tranquada (Brookhaven) <span style="float:right">M3B4</span>
  *Quantum magnetic excitations from stripes in cuprate superconductors*
  J. Zaanen (Leiden) <span style="float:right">M3B5</span>
  *How orderly is high Tc superconductivity?*

### Physics of f-electron materials III. (PCFES 7)

Organized by: V. Sechovský, G.H. Lander <span style="float:right">Room C</span>
  Y. Aoki (Tokyo) <span style="float:right">M3C1</span>
  *Time-reversal-symmetry-broken superconductivity in the filled skutterudite PrOs4Sb12*
  G. Hilscher (Vienna) <span style="float:right">M3C2</span>
  *Unconventional superconductivity and magnetism in CePt3Si*
  G. Santi (Aarhus) <span style="float:right">M3C3</span>
  *Coexistence of ferromagnetism and superconductivity in the strongly correlated transition metal compound ZrZn2*
  T. Suzuki (Hiroshima) <span style="float:right">M3C4</span>
  *Pressure-induced superconductor-insulator transition in chalcogenide spinel compounds*

### Magnetic quantum phase transitions and related phenomena

Organized by: D. Belitz <span style="float:right">Room D</span>
  J. Mydosh (Leiden) <span style="float:right">M3D1</span>
  *Nexus between quantum criticality and phase formation: the case of URh2Si2*
  M. Aronson (Michigan) <span style="float:right">M3D2</span>
  *Magnetic correlations near quantum critical transitions*
  P. Coleman (Piscataway) <span style="float:right">M3D3</span>
  *Quantum critical behavior in antiferromagnets*
  T. Vojta (Missouri-Rolla) <span style="float:right">M3D4</span>
  *Ferromagnetic quantum phase transitions*
  T. Senthil (Cambridge) <span style="float:right">M3D5</span>
  *Topological excitations and fractionalization at quantum phase transitions*
  D. Belitz (Oregon) <span style="float:right">M3D6</span>
  *Concluding discussion*

## Fluid interfaces
Organized by: J. Daillant                                        Room E
  P. Jungwirth (Prague)                                M3E1
  *Ions at the air/water interface*
  K. Mecke (Stuttgart)                                 M3E2
  *Microscopic structure of fluid interfaces*
  S. Mora (Orsay)                                      M3E3
  *Surface energy of liquid interfaces: an x ray synchrotron study*
  L. Rekvig (Trondheim)                                M3E4
  *Bending self-assembled amphiphilic monolayers*

## Carbon nano-tubes
Organized by: L. Kavan, H. Kuzmany                               Room F
  M. Damnjanovic (Belgrade)                            M3F1
  *Phonons in carbon nanotubes*
  C. Kramberger (Vienna)                               M3F2
  *Determination of chiral vectors in ultra thin carbon nanotubes by multi frequency Raman spectroscopy*
  J. Kurti (Budapest)                                  M3F3
  *Curvature effects in the electronic properties of small diameter single-walled carbon nanotubes*
  E. Obraztsova (Moscow)                               M3F4
  *Resonant character of Raman scattering in single-wall carbon nanotubes confirmed by photoluminescence measurements*
  T. Pichler (Dresden)                                 M3F5
  *Low-energy electronic structure of intercalated single wall carbon nanotubes*
  J.L. Sauvajol (Montpellier)                          M3F6
  *C60 excitations in Peapods : an inelastic neutron scattering investigation*
  C. Thomsen (Berlin)                                  M3F7
  *(n,m) chirality assignment based on Resonant Raman Scattering*

## Molecular dynamics studies of surfaces processes
Organized by: A. Fasolino                                        Room G
  A. Fasolino (Nijmegen)                               M3G1
  *Dynamics at surfaces: open questions and computational challenges*
  R. Ferrando (Genova)                                 M3G2
  *Simulation of surface diffusion*
  M. Kotrla (Prague)                                   M3G3
  *Submonolayer growth with impurities: Attractive vs. repulsive impurity-adatom interaction.*
  Z. Kuntova (Prague)                                  M3G4
  *Decay mechanisms of nanoislands - Monte Carlo simulations*
  U. Tartaglino (Trieste)                              M3G5
  *Surface friction, lubrication, and atomistic simulation*

## Nitrogen bonds and bands in diluted nitrides
Organized by: P. J. Klar                                                  Room H

E.P. O'Reilly (Cork)                                                      M3H1
*Theory of the electronic structure of dilute nitride alloys: beyond the band-anti-crossing model*
A. Polimeni (Roma)                                                       M3H2
*Probing the electronic properties of dilute nitrides by carrier localization and effective mass measurements*
S. Tomic (Daresbury)                                                     M3H3
*Band structure and laser characteristics of the Ga(In)NAs/GaAs QWs: comparison of the theory with experiment*
K. Volz (Marburg)                                                        M3H4
*Growth and Structural Characterization of (GaIn)(NAs)*
L. Rekvig (Trondheim)                                                    M3E4
*Bending self-assembled amphiphilic monolayers*

## Superconducting qubits
Organized by: G. L. Ingold                                                Hall J

T. Duty (Göteborg)                                                       M3J1
*Experimental studies of a Josephson charge qubit with RF-SET read-out*
C. Bruder (Basel)                                                        M3J2
*Transfer of quantum information through Josephson arrays*
E. Paladino (Catania)                                                    M3J3
*Telegraph and 1/f noise in Josephson qubits: decoherence and quantum control*
J. Pekola (Helsinki)                                                     M3J4
*Charge and flux controlled pumping of Cooper pairs*
J. Siewert (Regensburg)                                                  M3J5
*Adiabatic passage in superconducting nanocircuits*
M. Grifoni (Regensburg)                                                  M3J6
*Entanglement spectroscopy of a driven solid-state qubit and its detector*

## Poster Session 11:15–12:30

### Low dimensional systems

Sergey Reshetnyak                                                        S3X1
*Reflection of surface spin waves from semi-infinite uniaxial multilayer ferromagnetic structure*
A. Feher, A. Ya. Dulfan, P. A. Minaev, A. G. Shkorbatov, E. S. Syrkin   S3X3
*Resonance heat transport between two solids through multiplayer interface*
Antonio Hernandez-Cabrera, Pilar Aceituno, Fedir T. Vasko              S3X4
*Electron coherent dynamics after intersubband excitation*
M. Orlita, M. Byszewski, G. H. Dohler, R. Grill, S. Malzer, M. Zvara   S3X5
*Optical properties of indirect excitons in in-plane magnetic fields*
Pilar Aceituno, Antonio Hernandez-Cabrera,                             S3X6
*Trion dynamics in asymmetric coupled quantum wells*
Nataliya A. Goncharuk, Ludvi k Smrcka, Jan Kucera, Karel Vyborny       S3X7
*Comparison of semiclassical and quantum-mechanical description of 3D semiconductor superlattices subject to tilted magnetic fields*
Lev P. Avakyants, Pavel Yu. Bokov, Anatoly V. Chervyakov, Tamara P. Kolmakova   S3X8
*Photoreflectance from GaAs/GaAsP short period superlattices*

**Magnetism and strong correlations**

**Superconductivity**

**Biological physics**

**Theory**

Klaus Mecke, C. Mocuta, H. Reichert S3Z208
*Critical Dynamics: theory for time-dependent intensity correlations measured by X- ray microdiffraction*
A. Bainova, V. Arkhincheev S3Z209
*Non-maxwell charge relaxation: mechanisms and new nonexponential laws*
I.N. Adamenko, K.E. Nemchenko, I.V. Tanatarov S3Z210
*Energy flow density of a quasiparticle of a continuous medium with arbitrary energy-momentum relation*
K.A. Chalyy, L.A. Bulavin, A.V. Chalyi S3Z211
*Peculiarities of Critical Opalescence Spectrum in Liquids with Reduced Geometry*
Ihor Stasyuk, Oleg Vorobyov S3Z212
*The role of short-range interactions in one-dimensional proton conductor*
V. Arkhincheev S3Z213
*The generalization of Dykhne-Keller theorem for effective conductivity of random medium for a rhomb case.*
Lenka Zdeborova, Vaclav Janis S3Z214
*Mean-field theory of spin glasses: Replicated TAP free energy and its thermodynamic homogeneity.*
Y Muraoka, T Kasama, H Nishiyama, T Idogaki S3Z215
*Non-equilibrium Relaxation MC Study on the Phase Transition into the Partially Disordered State in the ANNNI Model*
L.K. Dash, N. Vast, P. Baranek, M.C. Cheynet, L. Reining S3Z216
*Ab initio spectra of the low-pressure phases of zirconia*
K.A. Chalyy S3Z217
*Cylindrically Confined Helium Heat Capacity: Theory Verification*
T. Frederiksen, M. Brandbyge, N. Lorente, A.-P. Jauho S3Z218
*Inelastic electron transport in metallic atomic wires*
Magdy Amin S3Z219
*The critical behaviour of the mean spherical model in the presence of three external fields*

**Chemical physics**

Jiri Vanicek, W.H. Miller S3Z220
*Quantum instanton calculation of isotopic effects on reaction rate constants*
Yasuhiro Senda, Fuyuki Shimojo, Kozo Hoshino S3Z221
*The phase transition of liquid phosphorus by ab-initio calculation*

# Thursday 22 July 2004

## Focused Sessions 8:30 – 10:00

Plasmonics with metal nanoparticles Room B
8:30 T. Klar (Mnchen) F4B1
*Metal nanoparticles as versatile nanotools: From optoelectronics to biophotonics*
9:00 J. Krenn (Graz) F4B2
*Nano-components for plasmonics*
9:30 V. Sandoghdar (Zürich) F4B3
*Microscopy, spectroscopy and manipulation of single gold clusters*

## Bose Half-metals for spintronics                                    Room C

8:30   R.A. de Groot (Nijmegen)                                        F4C1
       *Half-metals: defects and finite temperatures*
9:00   Z. Szotek (Daresbury)                                          F4C2
       *Transition metal oxide based half metals*

## Ferromagnetic superconductors                                       Room D

8:30   C. Pfleiderer (Karlsruhe)                                      F4D1
       *High pressure studies of superconducting band-ferromagnets*
9:00   A. Shick (Prague)                                              F4D2
       *Electronic structure and magnetic character of UGe2 and URhGe ferromagnetic
       superconductors*
9:30   S. Hayden (Bristol)                                            F4D3
       *Magnetism, superconductivity and heavy quasiparticles in ZrZn2*

## Solid/liquid interfaces                                             Room E

8:30   M. Reichling (Osnabrueck)                                      F4E1
       *Revealing the atomic structure of insulator surfaces*
9:00   A. Wieckowski (Urbana)                                         F4E2
       *Electrochemical interfaces studied by nuclear magnetic resonance of metals and
       metallized systems*
9:30   K. Wandelt (Bonn)                                              F4E3
       *Properties of metal/electrolyte interfaces*

## Nanotubes                                                           Room F

8:30   M. Remskar (Ljubljana)                                         F4F1
       *Synthesis, electron microscopy and applications of inorganic nanotubes*
9:00   J. Nygard (Copenhagen)                                         F4F2
       *Experiments on hybrid electronics incorporating carbon nanotubes*
9:30   J. Scott (Cambridge)                                           F4F3
       *Ferroelectric nanotubes and nano-ribbons*

## Giant piezoelectricity                                              Room G

8:30   R. Blinc (Ljubljana)                                           F4G1
       *Origin of giant electrostriction and piezoelectricity in relaxors*
9:00   X. Ren (Tsukuba)                                               F4G2
       *Giant electro-strain by point-defect-mediated reversible domain switching*
9:30   R.E. Cohen (Washington, D.C)                                   F4G3
       *Theory of polarization rotation in relaxor ferroelectrics*

## Microcavities                                                       Room H

8:30   W. Langbein (Dortmund)                                         F4H1
       *Microcavity polariton dynamics in the linear and non-linear regime*
9:00   L.S. Dang (Grenoble)                                           F4H2
       *Polariton stimulation and condensation in semiconductor microcavities*

## Structural studies of lowdimensional nanostructures — Hall J

8:30 K. Temst (Leuven) — F4J1
*Magnetization reversal in magnetic nanostructures studied by neutron reflectivity*
9:00 V. Holý (Prague) — F4J2
*Limits and prospects of X-ray scattering from self-organized epitaxial nanostructures*

## Plenary Session 10:30 – 12:30 — Hall A

10:30 T. Dietl (Warsaw) — P4A1
*Magnetic Semiconductors*
11:15 Agilent Technologies Europhysics Prize CEREMONY
11:45 D. Esteve (Saclay) — P4A2
*LAUREATES LECTURE: Towards superconducting quantum bit circuits*

## Mini–Colloquia 14:00 – 16:00

### Novel phenomena inatomic quantum gases
Organized by: F. Sols — Room B
J.H. Denschlag (Innsbruck) — M4B1
*Bose-Einstein condensation of 6Li2 molecules and the BEC-BCS crossover*
M. L. Chiofalo (Pisa) — M4B2
*Resonance effects on the crossover of bosonic to fermionic superfluidity*
A. J. Leggett (Illinois) — M4B3
*Overview*
J.Schmiedmayer(Heidelberg) — M4B4
*Atomic condensates near nanostructured surfaces*

### Physics of f-electron materials IV. (PCFES 7)
Organized by: V. Sechovský, G.H. Lander — Room C
A. Bianchi (Rossendorf) — M4C1
*Avoided Antiferromagnetic Order and Quantum Critical Point in CeCoIn5*
T. Hotta (Tokai) — M4C2
*Microscopic approach to superconductivity and magnetism of 115 compounds based on a j-j coupling scheme*
N. Metoki (Tokai) — M4C3
*Magnetic structure of UTGa5 and NpTGa5*
J. Paglione (Toronto) — M4C4
*Heat and charge transport at field-tuned quantum critical point*

### Role of spin in quantum transport
Organized by: V. I. Falko — Room D
D. Frustaglia (Pisa) — M4D1
*Conditions for adiabatic spin transport in disordered systems*
Y. Nazarov (Delft) — M4D2
*Role of nuclear spins in quantum dots*
J. Fabian (Graz) — M4D3
*Magnetic bipolar transistor*

## Entropic forces

Organized by: R. Roth | Room E

L. Helden ( Stuttgart) | M4E1
*Depletion forces in purely entropic systems*

A.A. Louis (Cambridge) | M4E2
*Polymer-colloid mixtures: the dark hand of entropy*

D.G.A.L. Aarts (Utrecht) | M4E3
*The interface in a phase separated colloid-polymer mixture*

## Interaction of matter with laser light under extreme conditions

Organized by: B. Rus | Room F

P. Nickles (Berlin) | M4F1
*Particle acceleration from laser-created relativistic plasmas*

D. Batani (Milano) | M4F2
*Equation of state measurements and phase transitions in the megabar regime with laser-driven shock waves*

D. Ros (Paris) | M4F3
*Interferometry applications of X-ray lasers at LIXAM. Diagnostics of surfaces and plasmas using X-ray lasers. Recent progress and perspectives : towards to the future LASERIX facility of LIXAM*

G. Tallents (York) | M4F4
*The production of extreme ultra-violet laser radiation by optical laser irradiation of solid targets*

## Structure and dynamics of disordered ferroelectrics

Organized by: J. Petzelt, J. Hlinka | Room G

A. Bussmann-Holder (Stuttgart) | M4G1
*The microscopic origin of relaxor ferroelectricity*

J.-M. Kiat (Paris) | M4G2
*Morphotropic phases in PSN-PT : bulk and thin film*

V. Shvartsman (Aveiro) | M4G3
*Investigation of polar structure in PMN-PT relaxors via Piezoresponse Force Microscopy*

Y. Uesu (Tokyo) | M4G4
*Soft mode behaviors in induced ferroelectric states in quantum paraelectric $SrTiO3$ and $KTaO3$*

T. Egami (Tennessee) | M4G5
*Lattice dynamics of relaxor ferroelectrics*

R. Blinc (Ljubljana) | M4G6
*Disorder and phase transitions in classical perovskites and relaxors*

W. Kleemann (Duisburg) | M4G7
*Structure and dynamics of uniaxial relaxor ferroelectrics*

S. Kamba (Prague) | M4G8
*Phonons and central mode behaviour in $PbMg1/3Nb2/3O3$ and $PbSc1/2Ta1/2O3$ relaxor ferroelectrics*

M. Glogarova (Prague) | M4G9
*Liquid crystalline phases formed by nonchiral bent-shaped molecules*

## Ultrafast spectroscopy

Organized by: J. -Y. Bigot                                        Room H

N. Del Fatti (Talence)                                           M4H1
*Electron - phonon scattering and acoustic vibrations in metal clusters*

P. Gilliot (Strasbourg)                                          M4H2
*Electron-hole relaxation dynamics and time-resolved optical- phonon emission in ZnCdTe quantum wells and quantum*

A. Kirilyuk (Nijmegen)                                           M4H3
*Ultrafast Spin Dynamics in Antiferromagnetic Materials*

P. Nemec (Prague)                                                M4H4
*Tailoring ultrafast carrier dynamics in CdSe and CdS nanocrystalline films prepared by chemical bath deposition*

I.E. Perakis (Heraklion Crete)                                   M4H5
*Ultrafast light-induced magnetization dynamics in III-V ferromagnetic semiconductors*

E. Peronne (Paris)                                               M4H6
*Ultrafast acoustics*

M. Vomir (Strasbourg)                                            M4H7
*Time dependant ferromagnetic resonance induced by femtosecond optical pulses in Co films*

J.A. Davis (Cambridge)                                           M4H8
*Time-resolved degenerate four-wave mixing (TR-DFWM) of magneto-excitons in GaAs/AlGaAs single quantum wells*

## Quantum decoherence and dissipation in mesoscopic system

Organized by: M. Grifoni, U. Weiss                               Hall J

G. Falci (Catania)                                               M4J1
*Interaction of Josephson qubits with strong QED cavity modes: dynamical entanglement transfer and navigation*

H. Grabert (Freiburg)                                            M4J2
*The quantum Smoluchowski equation*

D. Haviland (Stockholm)                                          M4J3
*Tunable quantum fluctuations with Josephson SQUID arrays*

J. Peguiron (Regensburg)                                         M4J4
*Duality relation for quantum ratchets*

M. Thorwart (Dsseldorf)                                          M4J5
*Macroscopic quantum effects in a strongly driven nanomechanical resonator*

## Poster Session 16:00–18:00

**Magnetism and strong correlations**

Andrey L. Kutepov                                                S4X1
*Electronic and Magnetic Structure of Pu, Am, and Cm*

Abdessamad Abada, Bahia Si-Lakhal                                S4X2
*Sum rules for four-spinon dynamic structure function in antiferromagnetic heisenberg model*

A. Sherman, M. Schreiber                                         S4X3
*Resonance peak and incommensurability in cuprate perovskites*

Z.V. Popovic, A. Cantarero, W.H.A. Thijssen, N. Paunovic, Z. Dohcevic-Mitrovic, F. Sapina                                                          S4X4
*Orbital ordering in B-site doped manganites*

M. Deppe, H. S. Jeevan, R. Borth, N. Oeschler, O. Stockert, C. Geibel, F. Steglich S4X26
*Magnetism and superconductivity in $CeCu_2(Si_{1-x}Ge_x)_2$*
M. Sikora, B. Sobanek, C.J. Oates, M. Borowiec, D. Zajac, D. Rybicki, B. Majcher, Cz.
Kapusta, C. Autret, K. Knizek, Z. Jirak, F. Bondino, M. Zangrando, C. Marquina S4X27
*XANES study of Mn and Co valence state in LaMn1-xCoxO3*
G. Chaboussant, H.U. Guedel, B. Barbara, A. Mueller, H. Mutka S4X28
*Quantum spin state mixing in frustrated nanomagnets*
A.V. Kolomiets, T. Goto, Y. Yoshida, S.-I. Ikeda S4X29
*Pressure effect on multiple metamagnetic transitions in $Sr_3Ru_2O_7$.*

**Semiconductors**

Cestmir Drasar, Petr Lostak, Jeffrey S. Dyck, Ctirad Uher S4X30
*Novel diluted magnetic semiconductors $Sb_{2-x}V_xTe_3$ and $Sb_{2-y}Cr_yTe_3$* P. Dziawa, B. Taliashvili, V. Domuchowski, E. Lusakowska, I. Demchenko, K. Dybko, M. Arciszewska, W.
Dobrowolski, V. Osinniy, A. Nadolny, T. Story S4X31
*MBE growth and characterization of EuGdTe ferromagnetic semiconductor*
Evgeny Z. Meilikhov, Rimma M. Farzetdinova S4X32
*Generalized mean-field theory of semiconductors and metals with magnetic*
Diego Frustaglia, Juergen Koenig, Allan H. MacDonald S4X33
*Spin Waves in Diluted-Magnetic-Semiconductor Quantum Wells*
N. Guerfi S4X34
*Oxidation of thin films of $TaSi_2$ and $WSi_2$ prepared on polycrystalline Si*
C. Michel, P.J. Klar, S.D. Baranovskii, P. Thomas, W. Heimbrodt S4X35
*Theory of magnetotransport in magnetic semiconductors and hybrid structures*
S. Ye, P.J. Klar, W. Heimbrodt, M. Lampalzer, W. Stolz S4X36
*Magnetotransport in GaMnAs/MnAs paramagnetic-ferromagnetic hybrids*
E. Skipetrov, M. Mikheev, O. Volkova, A. Plastun, F. Pakpour, V. Slynko S4X37
*Magnetic properties of diluted magnetic semiconductors $Pb_{1-x}Ge_xTe:Cr$*
J. Masek, F. Maca S4X38
*Ferromagnetic exchange coupling in n-type doped (Ga,Mn)As*
T. Andrearczyk, T. Dietl, K. Rode, A. Anane, R. Mattana, J.-P. Contour, O. Durand, R.
LeBourgeois S4X39
*Low Temperature Magnetoresistance of (Zn,Co)O Films*
Bimal Kumar Sarkar. S4X40
*Carrier-induced ferromagnetism in the nitrogen doped diluted magnetic semiconductor
Zn1-xMnxSe*
Young Mi Cho, Sang Soo Yu, Young Eon Ihm, Seung Won Lee, Hyojin Kim, Dojin Kim,
Jae Min Sohn, Bong Goo Kim, Young Hwan Kang S4X41
*Electrical and magnetic properties of neutron-irradiated polycrystalline Ge1-xMnx semiconductors grown by MBE*
C. Timm, A. H. MacDonald S4X42
*Anisotropic RKKY interactions in (Ga,Mn)As*
Jae Ho Sim, Hyun Jung Kim, Hyojin Kim, Woong Kil Choo S4X43
*Electrical and magnetic properties of Cr-doped ZnO thin films grown by reactive magnetron sputtering*
P.J. Klar, L. Chen, W. Heimbrodt, F. Brieler, M. Froeba, T. Kurz, H.-A. Krug von Nidda,
A. Loidl S4X44
*Modified magnetic properties of (II,Mn)VI in nanowires*

## Soft matter

## Optics

A. Kalvova, B. Velicky S4X64
*Disorder induced e-h correlation in phototransients in semiconductors*
J. Pejchal, N. Solovieva, M. Nikl, J. B. Shim, A. Yoshikawa, T. Fukuda, A. Vedda, M. Martini, D. H. Yoon S4X65
*Scintillation characteristics of Yb-doped YAlO$_3$*
N.N. Ilichev, E.D. Obraztsova, S.V. Garnov, S.E. Mosaleva S4X66
*Single-wall carbon nanotube suspension: 1.54 mkm nonlinear transmission and passive Q-switcher for self mode-locking in Er-glass laser*
E. Hulicius, T. Simecek, J. Oswald, J. Pangrac, R. Werner, C. Alibert, Y. Rouilard, S. Civis, Z. Chobola S4X67
*Tunable midinfrared semiconductor lasers for laser spectroscopy*
Filip Kadlec, Hynek Nemec, Petr Kuzel S4X68
*Phase-sensitive time-domain terahertz reflectometry*

**Materials science**

M. Hulman, P. Costa, M.L.H. Green, S. Friedrichs, H. Kuzmany S4X69
*Raman spectroscopy of single wall carbon nanotubes filled with semiconductors*
Ch. Arns, M. Knackstedt, Klaus Mecke, S4Y101
*Predicting physical properties of disordered media from a single tomographic image*
Jan Lancok, Miroslav Jelinek, Claudine Garapon S4Y102
*Influence of the oxygen pressure on films properties fabricated by laser ablation from doped GGG single crystal target*
V.Yu. Bardic, M.F. Ledney S4Y103
*Connection of elastic properties for fullerene systems with intermolecular potential parameters*
S. Zadvorkin, E. Gorkunov, S. Grachev, S. Smirnov, V. Somova, M. Solomein S4Y104
*Physico-mechanical properties of plastically deformed carbon steels*
A.A. Yusupov, I. Djabbarov, M.K. Salakhitdinova S4Y105
*The influence of diversion from stoichiometry on heat conductivity of aluminium-yttrium garnet.*
Nadia Mamede Jose, Luis Antonio Sanchez de Almeida Prado, Inez Valria Pagotto Yoshida
*Cross-linking of silanol-terminated PDMS with multi-functional alkoxide precursors monitored by Small Angle X-Ray Scattering.*
M. Ledinsky, L. Fekete, S. Honda, T. Mates, A. Fejfar, J. Kocka S4Y107
*Evaluation of crystallinity of mixed phase silicon thin films from Raman scattering spectra*
K.G. Saw S4Y108
*Exploring the validity of the charged cluster model for chemical vapour deposition diamond growth*
M. Milnera, H. Vinzelberg, I. Moench, B. Zhao, A. Leonhardt, B. Buechner S4Y110
*CVD Synthesis and Transport Properties of Ferromagnetic Metal Filled Multiwall Carbon Nanotubes*
Osman Adiguzel S4Y111
*Smart materials and microstructural transitions in copper based shape memory*
Srdjan Tadic, Radmila Lucic, Milan Jovanovic S4Y112
*High-Temperature Deformation Behaviour of Ti3Al-Nb Intermetallic*
Kazutaka Terashima, Suzuka Nishimura S4Y113
*Future material system for OEIC; GaN on Si*
S. Francoual, M. de Boissieu, F. Livet, F. Yakhou, F. Bley, R. Caudron, J. Gastaldi S4Y114
*Dynamics of phason fluctuations in the i-AlPdMn quasicrystal*

S.V. Terekhov, P. Teredesai, A.V. Osadchy, E.D. Obraztsova, J.L. Yarger, H.D.Hochheimer
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*Pressure-induced effects in raman spectra of hipco nanotubes*
K. Brinkman, D. Su, A. Tagantsev, N. Setter S4Y139
*The Dielectric Response of Ordered and Disordered $Pb(Sc_{1/2}Ta_{1/2})O_3$ Thin Films*
Nicola Manini, A. Bordoni, P. Gattari, M. Lueders, E. Tosatti S4Y140
*Hund's rule Magnetism in $C_{60}$ ions?*
N. Manini, P. Gattari, E. Tosatti S4Y141
*Jahn–Teller Spectral Fingerprint in Molecular Photoemission: $C_{60}$*
A.O. dos Santos, M.A. Mota, F.C. Nascimento, A.A. Coelho, S. Gama, L.P.Cardoso S4Y142
*Structural characterization of the $PrNi_5$ compound by x-ray multiple diffraction*
R. Moret, P. Launois, T. Wagberg, B. Sundqvist, V. Agafonov, V.A. Davydov, A.V. Rakhmanina
S4Y143
*C60 dimerization under pressure : a combined x-ray/Raman study*
Tatiana Makarova S4Y144
*Magnetism in polymerized fullerenes*
Zdenek Matej, Viktoria Cherkaska, Radomir Kuzel S4Y145
*Real structure analysis of nanocrystalline and submicrocrystalline materials using X-ray diffraction*
B. Pedrini, J. L. Gavilano, H. R. Ott, S. Wessel S4Y146
*Haldane state versus magnetic order in alkali metal pyroxenes*
J. Pelcova, I. Stulikova, B. Smola S4Y148
*Phase transformation investigation in Mg - rare earth based alloys by electrical resistometry*
O.E. Kvyatkovskii, M.G. Shelyapina, I.B. Zakharova , A.L. Shelankov , T.L. Makarova
S4Y149
*Magnetism in Polymerized Fullerenes: Theoretical Study*
A.V. Malkov, V.B. Malkov, O.V. Malkov, V.G. Pushin, B.V. Shulgin S4Y150
*Defect state of the lattice of thin-film selenium crystals described by Riemann curvature*
J. Fedotova, A. Ilyuschenko, T. Talako, A. Belyaev, A. Letsko, J. Stanek S4Y151
*Effect of Al contents and annealing on B2 FeAl studied by TMS and XRD*
T.M. Saliev, M.S. Saidov, I.G. Atabaev, M.Kh. Ashurov S4Y152
*Investigation of structure of diamond C/Si heterojunction by scanning electron microscopy*

**Surfaces and interfaces**

Ernst Pijper, Annalisa Fasolino S4Z201
*Quantum dynamics of a dimer in a periodic potential*
I. E. Onosov, V. I. Visotskii S4Z202
*The influence of local changes of the STM resolution on the informative content of STM-images.*
A Shokouhy, M Ghoranneviss, M Gholipur Shahraky , A.H Sari, M.R Hantezadeh, S.H Haji Hosseini G S4Z203
*Topographical characterization of Nitrogen bombarded Ti6Al4V with plasma ion source using AFM*
L.A. Kizman, T.Yu. Popik, V.M. Feyer, O.B. Shpenik, Yu.V. Popik S4Z204
*Low-energy electron spectroscopy of GaAs*
I. Batko, M. Batkova S4Z205
*Utilisation of calorimetric tunneling experiments in condensed matter physics*
I. E. Onosov, V. I. Visotskii S4Z206
*Probe microscopy in using resonance tunneling*

J. L. Rodriguez-Lopez, J. M. Montejano-Carrizales, Umapada Pal , J. F. Sanchez- Ramirez, H. E. Troiani, D. Garcia, M. Miki-Yoshida, M. Jose-Yacaman                S4Z207
*Surface Reconstruction Improves Free Energy of Bimetallic Nanoparticles*
Rouven Luescher, Mehmet Erbudak, Refik A. Kortan, Yves Weisskopf                S4Z208
*Thin Al films on quasicrystalline Al-Pd-Mn: The impact of structural affinities on the crystal-quasicrystal interface.*
Ye. V. Syrnikov, V. N. Grigorev, V. A. Maidanov, A. A. Penzev, E. Ya. Rudavskii, A. S. Rybalko                S4Z209
*Concentration dependence of the diffusion coefficient in separating 4He-3He solid mixtures*
N. Kern                S4Z210
*Schottky and ohmic contacts*
A. Morgante, A. Cossaro, D. Cvetko, G. Bavdek, L. Floreano, R. Gotter, F. Evangelista, A. Ruocco                S4Z211
*CuPhtalocyanine-Au(110) interface formation.*
S. D. Wang, M. N. Chang, C. Y. Chen, T. F. Lei                S4Z212
*An Investigation of Breakdown Spots in Silicon Dioxide Film by Scanning Capacitance Microscopy*
Bruce M. Law, Jae-Hie J. Cho, Franccois Rieutord                S4Z213
*Dipole-dependent slip at smooth solid/liquid surfaces*
Mikael Borg, Catherine Stampfl, Anders Mikkelsen, Johan Gustafson, Edvin Lundgren, Jepser N. Andersen, Matthias Scheffler                S4Z214
*Phase diagram of Al-Na surface alloys from first principles*]
N.-T.H. Kim-Ngan, W. Soszka, Z. Tarnawski, A. Kozlowski                S4Z215
*Characterization of the metal-insulator phase transition of $Fe_{3(1-\delta)}O_4$ surfaces.*
C. Fusco, A. Fasolino                S4Z216
*Load dependence of atomic-scale friction on graphite: dynamical effects on the tip motion*
Claudio Fusco, Annalisa Fasolino                S4Z217
*Diffusion and nonlinear dynamics of adatoms and dimers on periodic surfaces*
F. E. Ghodsi, M Mafakheri, A. Novinrooz                S4Z218
*Microstructural and optical characterization of sol-gel derived $Al_2O_3$ thin films deposited by dip coating technique*
Yaroslav V. Filipov, V. S. Staschuk, V. A. Odarich                S4Z219
*Ellipsometry study of aluminum mirrors made by diamond microgrinding in a wide spectral range*
Viktor Dudr, Natalia Tsud, Stanislav Fabik, Martin Vondracek, Vladimir Matolin, Vladimir Chab, Kevin C. Prince                S4Z220
*Valence charge fluctuations in the ( $\sqrt{3} \times \sqrt{3}$) - Pb/Si(111) system.*
A. Shcharbakova                S4Z221
*Investigation of phase trasnformations in Ti/Si and Cu/Tin/Si system by plasma treatment*
V. Sandomirsky, A. V. Butenko, A. Ronen, R. Kahatabi, Y. Schlesinger                S4Z222
*Fermi Glass Behavior of Highly Resistive Thin PbTe films*
W. Soszka, D. Sitko, G. Jago, N.-T.H. Kim-Ngan, D. Goc-Jago, A. Wikarjak, G.Galas                S4Z223
*Investigations of electrical proprieties of single crystalline $BaTiO_3$ by means of low-energy ion spectroscopy*
I. Bartos, M.N. Read                S4Z224
*Surface resonances in VLEED*
Pingo Mutombo, Pavel Shukrinov, Vladimir Chab                S4Z225
*Experimental and theoretical characterization of Cu adsorption sites on a Si (111)- 7x7 surface*
C. González, P.C. Snijders, J. Ortega, R. Pérez, F. Flores, S. Rogge, H.H. Weitering S4Z226
*Formation of atom wires on vicinal silicon: Ga/Si(112)-(6x1)*

# Friday 23 July 2004

## Focused Sessions 8:30 – 10:00

Nanoscale materials                                              Room B

| | | |
|---|---|---|
| 8:30 | V. Vitek (Philadelphia) | F5B1 |
| | *From atomic structure of dislocations to deformation behaviour on all scales* | |
| 9:00 | L. Kubin (Paris) | F5B2 |
| | *From dislocations to strain hardening in fcc crystals: simulations and modelling* | |
| 9:30 | R. Wuerschum (Graz) | F5B3 |
| | *Diffusion and free volumes in nanoscaled materials* | |

Spin polarized transport                             Room C

| | | |
|---|---|---|
| 8:30 | N. Garca (Madrid) | F5C1 |
| | *Recent results on ballistic magnetoresistance: reproducibility, measurements in different laboratories and electrical effects* | |
| 9:00 | F. Montaigne (Nancy) | F5C2 |
| | *Parabolic band model for magnetic tunnel junctions and related devices* | |
| 9:30 | W. Van Roy (IMEC Leuven) | F5C3 |
| | *Spin injection into semiconductors through AlOx, Schottky, and Zener tunnel junctions* | |

Dilute Magnetic Semiconductors (DMS)              Room D

| | | |
|---|---|---|
| 8:30 | J. Kudrnovsky (Prague) | F5D1 |
| | *Exchange interactions in diluted magnetic semiconductors: first-principles study* | |
| 9:00 | T. Schulthess (Oak Ridge) | F5D2 |
| | *Valence and p-d exchange coupling of Mn impurities in III-V semiconductors* | |
| 9:30 | T. Jungwirth (Prague) | F5D3 |
| | *Magneto-transport in ferromagnetic (III,Mn)V semiconductors* | |

Self assembling networks: Ferrofluids, biological gels, and polymers Room E

| | | |
|---|---|---|
| 8:30 | G.J. Vroege (Utrecht) | F5E1 |
| | *Structure formation in iron ferrofluids* | |
| 9:00 | G. Porte (Montpellier) | F5E2 |
| | *Self assembling polymer microemulsion gels* | |

Quasicrystal surfaces as templates for the growth of quasiperiodic systems of reduced complexity                                        Room F

| | | |
|---|---|---|
| 8:30 | R. McGrath (Liverpool) | F5F1 |
| | *Pseudomorphic growth of a single element quasiperiodic ultrathin film on a quasicrystal substrate* | |
| 9:00 | R. Diehl (University Park) | F5F2 |
| | *The effect of aperiodic symmetry on thin film growth: Xe on Al-Ni-Co* | |
| 9:30 | W. Theis (Berlin) | F5F3 |
| | *Single element Sb and Bi quasiperiodic monolayers on quasicrystal surfaces* | |

## Hybrid biogenic and inorganic nanostructures          Room G

8:30    P. Fromherz (Garching)          F5G1
        *Semiconductor chips with ion channels, nerve cells and brain tissue*
9:00    P. Christianen (Nijmegen)          F5G2
        *Magnetic field manipulation of functional materials*

## Slow light          Room H

8:30    R.W. Boyd (Rochester)          F5H1
        *Slow and fast light in room temperature solids*
9:00    S. Odoulov (Kiev)          F5H2
        *Slow light propagation in photorefractive crystals*

## Quantum computing and decoherence          Hall J

8:30    H. Mooij (Delft)          F5J1
        *Coherent quantum dynamics of superconducting flux qubit*
9:00    J. Ankerhold (Freiburg)          F5J2
        *MQT read–out of Josephson junction qubits*
9:30    G. Ithier (Saclay)          F5J3
        *Analysis of decoherence of a superconducting quantum bit*

## **Plenary Session 10:30 – 12:30**          Hall A

10:30   M. Chan (University Park)          P5A1
        *Thermodynamic Casimir Forces*
11:15   I. Bloch (Munich)          P5A2
        *Exploring quantum matter in optical lattice potentials*
12:00   Conference closing

# Plenary Session 8:20 – 10:00      Hall A

P1A1    **Quantum Dot Nanostructures: Paradigm Changes in Semiconductor Physics**

Dieter Bimberg[1]

*1) Institut fr Festkrperphysik, TU Berlin, Germany*

Universal self organisation and self ordering effects at surfaces of semiconductors lead to the formation of coherent zero-dimensional clusters called quantum dots (QDs). A total energy model to explain the hierarchy of ordering is presented . The electronic and optical properties of QDs, being smaller than the de-Broglie-wavelength in all three directions of space, are closer to those of atoms in a dielectric cage than of solids. QDs possess a delta-function like density of states, and excitons show an extremly long low temperature phase relaxation time. Their energy eigenstates are only twofold degenerate and do not depend on momentum, which is no conservable any more. All many particle states are strongly Coulomb correlated. Many particle energies depend on shape and size of the dots, such that negative biexciton binding energies appear and no "free"electron-hole-pairs exist. There is no position independent Fermi-level at low temperatures. Static and dynamic properties of QD-based devices are described by Master equations of microstates, rather than by rate equations of averaged ensembles. Quantum dots can be exploited for novel optoelectronic devices, like lasers, amplifiers, single photon sources ... Record low lasing threshold or close to zero temperature sensitivity of the lasing threshold is found e.g. at the important communication wavelength of 1300 nm. Their emission wavelength can be tuned by varying only the geometry of the dot rather than its chemical composition. Thus the geometry of the nanostructure becomes the decisive design tool for new emission wavelengths enabling novel applications like semiconductor-laser-based TV or inexpensive solid state single photon sources for quantum cryptography. Nanotechnologies transform presently to enabling technologies for new economies. It is expected that first commercialisation of nanophotonic devices and systems will appear soon.

P1A2    **Spintronics**

A. Fert[1], M. Anane[1], A. Berthelemy[1], V. Cros[1], J-M. George[1], J. Grollier[1], H. Jaffres[1], J-L. Maurice[1], F. Peroff[1], P. Seneor[1], F. Van Dau[1]

*1) Unite Mixte de Physique CNRS/Thales and Universite Paris Sud*

Manipulating spin currents in nanostructures associating magnetic and nonmagnetic materials is the basic idea of spintronics, in contrast to mainstream electronics in which the spin of the electron is ignored. After an introduction on the basic concepts, the first steps of spintronics (Giant Magnetoresistance, Magnetic Tunnel Junctions, etc) and its current applications (hard discs, MRAM), I will focus on some recent developments:
1) Spin transfer: The magnetic moment of a ferromagnetic element can be oriented without applying a magnetic field but only by transfusing spins carried by an electrical current. This is the concept of spin transfer. I will describe experiments in which the magnetization is coherently reversed by spin transfer and others in which the spin transfer is used to move back and forth a magnetic domain wall. Spin transfer is very promising for the switching of sub-micronic devices like MRAM.
2) Spintronics with semiconductors: Fusion between traditional electronics and spintronics in semiconductor/ferromagnetic heterostructures is a very attractive goal. I will summarize the recent advances in this field.
3) Nano-spintronics: Spin manipulation in quantum boxes (qubits) is the basis of several concepts of quantum computer. I will describe experiments combining spin injection into a nanoparticle and Coulomb blockade to probe the spin coherence in confined geometry.

# Focused Sessions 10:30 – 12:00

*Nanoscience at large facilities* **Hall A**

F1A1 **Order and disorder in magnetic nanostructures as studied by polarised neutron reflectometry**

Sean Langridge[1]
*1) Rutherford Appleton Laboratory, CCLRC*

Polarised Neutron Reflectometry (PNR) is ideally suited to the study of magnetic nanostructures. In this talk we shall discuss the use of polarised neutron scattering techniques to obtain absolute, quantitative information on the *intra* layer magnetic coupling and on the *in-plane* magnetic ordering from buried interfaces. We shall discuss examples of PNR studies of magnetic ordering (disorder) in spintronic and patterned systems and the new insight obtained.

Given the proposed developments in new neutron instrumentation we shall also highlight some of the potential future applications.

F1A2 **Photoelectron emission microscopy of magnetic domains in layered magnetic structures**

Wolfgang Kuch[1]
*1) Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany*

The fundamental investigation of layered magnetic structures, which exhibit a variety of new and interesting effects, calls for a method capable of delivering microscopic magnetic information for each of the several magnetic layers separately. Photoelectron emission microscopy (PEEM) with synchrotron radiation is such a technique. Based on the element selectivity of x-ray magnetic circular dichroism (XMCD), it allows for layer-resolved magnetic domain imaging. I will show examples of layer-resolved XMCD-PEEM studies performed at BESSY that proof the importance of a local magnetic interlayer coupling mechanism by magnetic stray fields from domain boundaries, and reveal the antiferromagnetic spin structure of ultrathin FeMn layers. An interesting aspect of XMCD-PEEM is the possibility for time-resolved stroboscopic measurements of the magnetization reversal dynamics exploiting the time structure of the synchrotron radiation.

F1A3 **Self-organized semiconductor quantum dots in the light of synchrotron radiation**

Till H. Metzger[1]
*1) ESRF. Grenoble, France*

In strained layer semiconductors, nano-sized islands (quantum dots) are formed after the deposition of a few layers of the dot material on a substrate with a different lattice parameter. Advanced X-ray diffraction methods using synchrotron radiation are perfectly suited to characterize the structural properties. We demonstrate how anomalous dispersion is combined with grazing incidence diffraction to determine the size, strain and chemical composition in nano-structures. Three examples will be presented: 1) Ge on Si, we show how the 3D chemical composition and the atomic ordering of the GeSi alloy forming the dots can be quantified. 2) From the intensity maps in reciprocal space, we reveal a highly anisotropic In distribution within InAs quantum rings formed after GaAs overgrowth. 3)First x-ray in-situ studies of islands evolving from ion erosion on GaSb are shown.

*Bose Einstein condensation in lowdimensional semiconductor* **Room B**

### F1B1 — Spontaneous Coherence in Bilayer Quantum Hall Systems

A.H. MacDonald [1]
*1) University of Texas at Austin*

Quantum Hall bilayer systems can have ground states with spontaneous interlayer phase coherence. Coherence has been revealed by surprising features observed in two different types of transport experiments, interlayer tunneling and counterflow conductivity. I will review the theoretical understanding of this broken symmetry state and explain its equivalence to excitonic Bose condensation. I will also discuss a theory which is able to account for most aspects of both experiments. This theory emphasizes the close relationship between these experiments and spin-transfer phenomena in ferromagnetic metals.

References: J.P. Eisenstein and A.H. MacDonald, Bose-Einstein Condensation of Excitons in Bilayer Electron Systems, cond-mat-0404113. A.S. Nunez and A.H. MacDonald, Spin Transfer Without Spin Conservation, cond-mat-0403710. M. Abolfath, A.H. MacDonald and L. Radzihovsky, Critical Currents of Ideal Quantum Hall Superfluids, Phys. Rev. B 68, 155318 (2003).

### F1B2 — Indications of excitonic superfluidy in a quantum Hall bilayer

I. B. Spielman[1], M. Kellogg[1], J. P. Eisenstein[1], L. N. Pfeiffer[2], K. W. West[2]
*1) California Institute of Technology*
*2) Lucent Bell Laboratories*

Superfluidity and the quantum Hall effects are separately among the most stunning macroscopic manifestations of quantum mechanics. Although generally occurring in different systems, a bilayer two dimensional electron system at high magnetic field can exhibit both. Our studies of the bilayer $\nu_T = 1$ quantum Hall state find evidence suggesting that it is simultaneously a quantum Hall system and an excitonic superfluid. At $\nu_T = 1$ the longitudinal resistance shows a deep minimum and the Hall resistance is quantized at $h/e^2$. Here I present several experimental results highlighting the superfluid properties of this state. First I present Coulomb drag measurements, and continue with interlayer tunneling data showing the development of a step-like tunneling $I$-$V$ strongly reminiscent of a Josephson discontinuity. I conclude with a direct detection of the predicted counter-flow superfluid mode, in which and $\rho_{xx}$, and $\rho_{xy}$ simultaneously approach zero.

### F1B3 — Evidence for a Superfluid Phase in a Solid below 20 K

P. Wachter[1], B. Bucher[1], J. Malar[1]
*1) Laboratorium für Festkörperphysik, ETH Zürich, 8093 Zürich, Switzerland*

At high pressures (up to 17 kbar) and low temperatures (1.5 K - 300 K) a condensed excitonic phase of intermediate valent $TmSe_{0.45}Te_{0.55}$ has been realized under equilibrium conditions. We have measured the heat conductivity $\lambda$, the thermal diffusivity $a$ and the longitudinal sound velocity $v$ as a function of pressure and temperature. The specific heat was inferred through $c_v \propto \lambda/a$ and thus could be obtained for the first time in a solid in the whole pressure and temperature range mentioned above.

We have given evidence that in the Bose condensed excitonic state an ever increasing heat conductivity exists below about 20 K with a tendency to become infinite for T $\rightarrow$ 0 K. We use the analogy with $^4$He II to postulate superfluidity in our material. The second sound seems to be responsible for an ever increasing $a$, the thermal diffusivity, below 20 K beyond the limit of surface scattering. These results are unprecedented and for the first time could mark the stable existence of a superfluid phase in a solid.

*Field tuned quantum criticality in 2 and 3D correlated electron systems* **Room C**

F1C1 **Field-tuned quantum criticality in heavy fermion systems**

Philipp Gegenwart[1]

*1) Max-Planck Institute for Chemical Physics of Solids*

We discuss a series of thermodynamic, magnetic and electrical transport experiments on the two heavy fermion compounds $CeNi_2Ge_2$ and $YbRh_2Si_2$ in which magnetic fields, $B$, are used to tune the systems from a non-Fermi liquid (NFL) into a field-induced FL state. Upon approaching the quantum critical point from the FL side by reducing $B$ we analyze the heavy quasiparticle (QP) mass and QP-QP scattering cross sections. For $CeNi_2Ge_2$ the observed behavior agrees well with the predictions of the spin-density wave (SDW) scenario for three-dimensional (3D) critical spin-fluctuations. By contrast, the observed singularity in $YbRh_2Si_2$ cannot be explained by the itinerant SDW theory for neither 3D nor 2D critical spinfluctuations.

Work done in collaboration with J. Custers, R. Küchler, F. Weickert, N. Oeschler, J. Ferstl, T. Cichorek, Y. Tokiwa, K. Neumaier, H. Wilhelm, J.A. Mydosh, C. Geibel, and F. Steglich

F1C2 **Open Issues in Field Driven Quantum Criticality**

A. J. Schofield[1]

*1) The University of Birmingham, United Kingdom*

The Hertz theory of the quantum critical point seems to be failing to account for the observed behaviour seen in a wide variety of quantum phase transitions. The origin of these failings is an area of active research. The use of a magnetic field to tune a material to a quantum critical point has allowed a detailed study of both quantum phase transitions and a new type of quantum criticality – the metamagnetic quantum critical endpoint. I will show how this latter example should be an ideal test case for the Hertz theory. Yet even in the itinerant metamagnet $Sr_3Ru_2O_7$ unusual behaviour is seen where the critical endpoint should be[1]. The challenge this poses for theory will be discussed. In the case of quantum criticality in heavy fermion systems tuned by a magnetic field there is evidence that a Fermi surface volume change is taking place[2]. Efforts to develop the theory for this observation will be reviewed.

[1] R. S. Perry *et al*., cond-mat/0401371. [2] S. Paschen *et al.*, to be published.

F1C3 **Quantum Criticality in 2 layer Strontium Ruthenate**

Andrew Mackenzie[1]

*1) University of St. Andrews, Scotland*

In this talk I will describe work being done by several groups to investigate the consequences of tuning the critical end-point of a line of first-order metamagnetic transitions towards zero temperature. Particular attention will be paid to dramatic changes in the properties in the vicinity of the transition as the purity of the crystals is increased.

*Dynamical Mean Field Theory for real materials* **Room D**

F1D1  **Realistic modelling of materials with strongly correlated electrons**

D. Vollhardt[1]

*1) Theoretical Physics III, University of Augsburg, D-86135 Augsburg, Germany*

In the last few years a remarkable fusion of conventional band structure theory and many-body theory, based on the dynamical mean-field theory (DMFT), has taken place. In particular, the LDA+DMFT approach has been successfully employed to calculate **k**-integrated spectra of various transition metal oxides such as $V_2O_3$ and $(Sr,Ca)VO_3$, making a comparison with spectroscopy experiments possible. I will discuss recent insights into the nature of the Mott–Hubbard metal–insulator transition in $V_2O_3$ obtained by this approach, e.g., the influence of the orbital degrees of freedom on the transition, and the filling of the Mott gap with increasing temperature. Furthermore, I will comment on generalizations of the LDA+DMFT scheme which allow one to calculate also **k**-resolved spectral functions and thus predict ARPES spectra. Finally, a new, fully *ab-initio* and self-consistent formalism for calculating the electronic structure of strongly correlated materials, based on Wannier functions, will be discussed.

F1D2  **Electronic structure calculations for correlated materials – some recent advances on transition metal compounds**

Silke Biermann[1], Alexander I. Poteryaev[2], Alexander I. Lichtenstein[3], Antoine Georges[1]

*1) CPHT, Ecole Polytechnique, 91128 Palaiseau, France*
*2) University of Nijmegen, NL-6525 ED Nijmegen, The Netherlands*
*3) Universität Hamburg, Germany*

During the last years new methods for the description of the electronic structure of correlated materials have been developed. The combination of dynamical mean field techniques with density functional theory allows for the calculation of electronic properties of materials from first principles, including strong Coulomb interactions. We will describe some recent advances on transition metal compounds[1,2], in particular on $VO_2$ [3].

[1] E. Pavarini, S. Biermann, A. Poteryaev, A. Lichtenstein, A. Georges, O. K. Andersen, Phys. Rev. Lett. **92**, 176403 (2004).
[2] F. Lechermann, S. Biermann, A. Georges, in preparation.
[3] S. Biermann, A. Poteryaev, A. Lichtenstein, A. Georges, in preparation.

*Magnetic field effects in cold glasses* **Room E**

### F1E1 __Dephasing of Atomic Tunneling by Nuclear Quadrupoles__

Alois Wuerger[1]

*1) CPMOH, CNRS-Universite Bordeaux 1, 351 cours de la Liberation, 33405 Talence, France*

Recent experiments on tunneling systems in insulating glasses showed an unexpected magnetic-field dependence of spontaneous polarization echoes. Besides a strong overall increase with the magnetic field, the echo amplitude slowly oscillates with a frequency that is proportional to the magnetic field. We have developed a theory that couples the tunneling motion to nuclear quadrupoles and obtain the beat frequency and dephasing in terms of the nuclear magnetic and quadrupolar moments, the waiting time, and the magnetic field [A.W., C. Enss, A. Fleischmann, Phys. Rev. Lett. 89, 237601 (2002)]. Our results compare favorably with measurements on various amorphous solids.

### F1E1 __Influence of Nuclear Spins on the Low Temperature Properties of Glasses__

Christian Enss[1]

*1) Physics Department, Brown University, BOX 1843, Providence, RI, USA*

A few years ago strong magnetic field effects have been observed in low-temperature dielectric susceptibility measurements and in coherent polarization echo experiments on certain glasses and disordered crystals. The low-temperature dielectric properties of such materials are dominated by atomic tunneling systems. It has been suggested that the surprising magnetic field dependence is caused by tunneling particles with nuclear quadrupole moment. For such systems there exists a coupling of the tunneling motion with the nuclear quadrupole moments experiencing the electric field gradients in the localized states. This coupling gives rise to a quadrupole splitting of the energy levels of the tunneling systems. The applied magnetic field then leads to an additional Zeeman splitting of the nuclear levels. We review the results of polarization echo experiments in magnetic fields and discuss the role of the nuclear spins in such experiments.

### F1E3 __Magnetic field effects of the dielectric properties of disordered solids__

Georg Weiss[1]

*1) Physikalisches Institut, Universität Karlsruhe*

The low temperature thermal, acoustic, and dielectric properties of glasses are dominated by low energy excitations which are caused by the tunneling of small atomic clusters between two energetically almost equivalent sites. The characteristic variation with temperature of the dielectric susceptibility gives hope to develop a capacitance thermometer for temperatures well below 1K with the expected advantage of being not influenced, in principle, by an external magnetic field. It turns out, however, that the dielectric susceptibility of various silicate glasses, $SrTiO_3$ based glass ceramics, and doped alkali halides undergo quite strong non-monotonic changes as a magnetic field is applied. A review will be given on this unexpected behaviour which presently is not yet fully understood.

*Manipulations at surfaces*　　　　　　　　　　　　　　　**Room F**

F1F1　　**Mechanics of atomic manipulation and nano-pattern formation**

J.B. Pethica[1], H.O. Ozer[1], G. Cross[1], B. O'Connell[1], A. Norris[1]
*1) SFI Laboratory, Dept. of Physics, Trinity College Dublin*

The operating conditions for STM are known from recent AFM measurements to involve considerable mechanical interaction between tip and sample even under so-called normal imaging conditions. This can lead to image distortion. It can also cause movement of atoms, both controllable and uncontrolled, and examples of both will be shown. The onset of energy dissipation (atom friction) prior to permanent atom displacement can now be observed in AFM. Quantitative results from a new low amplitude AFM will be presented. The second part of the talk will describe recent results from instrumented indentation in polymer thin films for nano-imprint lithography. This allows assessment of the geometry and strain state during the imprint process as well as after production of the net shape. The archetypal geometries of flat punch (for vias) and cavity (for mesas) will be shown, and the conditions for formation below Tg described. The problem of residual film thickness, or mask ratio, will be discussed.

F1F2　　**Controlled manipulation of atoms and molecules on surfaces**

Karl-Heinz Rieder[1]
*1) Free University of Berlin, Department of Physics, Arnimallee 14, D-14195 Berlin*

Recent progress in using the scanning tunneling microscope (STM) for manipulation of individual atoms and molecules is surveyed. Seasonal topics will be chosen from
- build-up of artificial nanostructures and determination of their properties
- role of tip-particle forces in soft manipulation (pulling, pushing, sliding)
- manipulation and contacting of complex molecules
- scattering of surface and interface electron waves
- vertical manipulation, physical reasons for the appearance of chemical contrast
- induction of all steps of chemical reactions with funcionalized tips
- investigation of vibrational and electronic influences upon electron induced processes
- molecular shooting: a novel manipulation process
- experiences with attempts to transfer manipulation techniques from metal surfaces to thin insulating films.

F1F3　　**A fresh STS look at surface states and single impurities on metals**

R Berndt[1], L Limot[1], J Kröger[1], E Pehlke[1], P Johansson[2]
*1) Universität Kiel, D-24098 Kiel, Germany*
*2) Örebro Universiteit, S-701 82 Örebro, Sweden*

In recent years, Scanning Tunnelling Microscopy (STM) and Spectroscopy (STS) have been used to image, manipulate and acquire the local density of states of adatoms on metal surfaces. We will first address differences that remain between STS results for noble metal surface states and related photoelectron spectroscopy data. Next, we will focus on the spectroscopy of Co-adatoms on Ag(111). Unlike non-magnetic adatoms, the tunnelling spectra obtained on and near some magnetic adatoms like Ce or Co yield a characteristic Fano line around the Fermi energy which is the signature of the Kondo effect. We will report STS data over a wider range of energies which we recorded in an attempt to better understand the interaction of adatoms with surface states.

*Topological defects in materials* **Room G**

**F1G1** **Isometric distortions in liquid crystals with simultaneous smetic and columnar order. Helicity and frustration.**

Maurice Kleman[1]
*1) Universit Paris 6. LMCP/CNRS*

Smectic or columnar liquid crystals present specific defect textures, due to the competition of curvature deformations (involving liquid relaxation) and strain (positional deformation). In fact, deformations in 1D and 2D LCs can show no strain at all (isometric distortions), especially on large scales! (*focal conic* domain in smectics; *developable domains* in columnar phases).
The observation of defects in the recently discovered bent-core molecule LC phases has considerably enlarged the scope of possible isometric distortions, because some of these phases are simultaneously smectic, columnar, and chiral (a feature in principle incompatible with smectic ordering) [Yu.A. Nastishin, M.F. Achard, H.T. Nguyen, M. Kleman. Eur. Phys. J. E12 581 (2003)]. We discuss the resulting (double-) *helical ribbon* textures, which are frustrated, isometric, distortions.

**F1G2** **Metadislocations in quasicrystal approximants**

Hans-Rainer Trebin[1], Michael Engel[1]
*1) Institut für Theoretische und Angewandte Physik, Stuttgart University, D-70550 Stuttgart*

The quasicrystalline alloy i-Al-Mn-Pd possesses as crystalline approximant the $\xi'$-phase, which is formed by parallel columns of Mackay-type clusters. Projection along the columns yields a pattern of staggered hexagons whose orientation can be reverted by phason-like defects. In $\xi'_n$-approximants these defects establish a periodic superstructure. Therein Klein et al. [PRL **82** 3468 (1999)] discovered "metadislocations" which are the mesoscopic textures of partial "lattice"-dislocations. We propose a scheme to construct the column-pattern of a series of approximants ($\xi$, $\xi'$, $\xi'_n$) and of their metadislocations by cuts and projections from a single higher-dimensional periodic lattice. An explicit relation is given between the Burgers vector of a lattice-dislocation and of the corresponding metadislocation. Combination mechanisms of the metadislocations are presented. Our studies are an example of how hyperspace methods from the theory of quasicrystals can be applied to get insight into the defect structure of crystalline complex metallic alloys.

**F1G3** **Role of topological defects in liquid crystals with dipolar order**

Lubor Lejček[1]
*1) Institute of Physics, Czech Academy of Sciences, Na Slovance 2, 182 21 Prague 8, Czech Republic*

Typical linear topological defects observed in ferroelectric (FE) or antiferroelectric (AF) liquid crystalline phases are dislocations and disclinations:
1) In chiral smectic C phase of liquid crystals with the phase transition cholesterics - chiral smectic C domains of rectangular-like shape, called twin-like domains, are observed which are mediated to outside region by dislocations.
2) In thicker FE samples with high value of spontaneous polarization twist disclinations are sources of the electrostatic charge which influences their existence.
3) Line defects called dispirations - combination of layer dislocations and director disclinations - were observed in AF phases of chiral smectic C liquid crystals.
4) In free-suspended chiral smectic C films cholesteric inclusions nucleate near the chiral smectic C - cholesteric transition and form linear chains.

*Single photon solid state sources* **Room H**

F1H1 **Single Photon Devices for Quantum Cryptography**

Andrew Shields[1]
*1) Toshiba Research Europe Ltd*

Quantum optics may soon provide a method to guarantee absolutely the secrecy of digital keys sent across optical fibres. I discuss here the constraints on practical QKD systems that operate over long fibres. In an optimal attack on such a system, an eavesdropper would target the multi-photon pulses inevitably generated by weak coherent sources. Preventing this attack restricts the maximum fibre length and bit rate. The development of true single photon sources is thus important for unconditionally secure quantum cryptography, as well as photonic implementations of quantum computing and other applications in quantum optics. A natural approach to realise practical single photon devices is to adapt conventional solid state light emission and detection technologies. I will discuss progress towards single photon generators based on integrating an InAs quantum dot into light emitting diodes, as well as how quantum dots can be used for low noise detection of single photons.

F1H2 **Quantum optical studies on quantum dots and on individual acceptor bound excitons in semiconductors**

S.M. Ulrich[1], M. Benyoucef[1], P. Michler[1], J. Wiersig[2], F. Jahnke[2], M. Kamp[3], A. Forchel[3], S. Strauf[4]
*1) 5. Physikalisches Institut, Universität Stuttgart, Stuttgart, Germany*
*2) Institut für Theoretische Physik, Universität Bremen, Bremen, Germany*
*3) Technische Physik, Universität Würzburg, Würzburg, Germany*
*4) Materials Department, University of California, Santa Barbara, USA*

In this talk we present recent results on triggered single-photon emission from single QDs and individual acceptor bound excitons in a semiconductor. Furthermore, we will report on the generation of linear polarization correlated photon pairs emitted by the radiative biexciton (XX)-exciton (X) cascade of a single QD. In addition, we demonstrate the possibility of using the XX-X radiative cascade of a single QD in a pillar microcavity to efficiently generate triggered photon pairs.

*Electron dephasing* **Hall J**

F1J1 **Low-temperature dephasing of quantum interference in mesoscopic systems**

Yoseph Imry[1]
*1) Weizmann Institute, Rehovot, Israel*

The conduction electrons' dephasing rate, $\tau_\phi$, is expected to vanish with the temperature. An intriguing apparent saturation of this dephasing rate was recently reported at very low temperatures *of the electrons*. The suggestion that this represents dephasing by zero-point fluctuations has generated both theoretical and experimental controversies. We start by proving that the dephasing rate must vanish at when $T$ approaches 0, unless a large ground state degeneracy exists. Further experiments by Ovadyahu demonstrate unequivocally that when strictly *linear* transport is used, the apparent low-temperature saturation of $\tau_\phi$ is eliminated. Another novel result of the experiments is that heavy nonmagnetic impurities (gold) in the samples produce, even in linear transport, a shoulder in the dephasing rate at very low temperatures. We explain this as due to low-lying local defects, whose dephasing rate vanishes in fact with $T$.

F1J3 **Quantum decoherence of electrons in the ground state: Persistent currents and weak localization**

Andrei D. Zaikin[1]
*1) Forschungszentrum Karlsruhe, Institut für Nanotechnologie,76021, Karlsruhe, Germany*

Electron-electron interactions in disordered conductors cause suppression of electron coherence beyond a finite length scale down to zero temperature [1,2]. This effect fundamentally restricts the ability of electrons to interfere and severely impacts ground state properties of mesoscopic conductors. In this talk I will review the present status of the field focusing on theoretical developments and, if time permits, also on the relation between theory and recent experiments performed with diffusive metallic wires, carbon nanotubes and semiconducting structures.

[1] P. Mohanty, E.M.Q. Jariwala, and R.A. Webb, Phys. Rev. Lett. **78**, 3366 (1997).
[2] D.S. Golubev and A.D. Zaikin, Phys. Rev. Lett. **81**, 1074 (1998); Phys. Rev. B **59**, 9195 (1999).

# Mini-Colloquia 14:00 – 16:00

*Electronic entanglement and Bell inequalities in solid state systems*        **Room B**

### M1B1        **Entanglement in correlated electron systems**

A. Crépieux[1], R. Guyon[1], P. Devillard[1], T. Martin[1]
*1) Centre de Physique Théorique, Case 907, 13288 Marseille, France*

We review our results on correlated systems where electrons or quasiparticles are entangled. First, we consider a superconductor which is used as a source of entangled electrons[1]. This entanglement scenario is in close analogy with experiments in quantum optics which generate entangled photons using non linear crystals. Next, we consider a carbon nanotube which is described as a Luttinger liquid with two opposite chiralities. Electron injection in such nanotube leads to the propagation of entangled quasiparticles whose charges are related to the Luttinger liquid interaction parameter[2].

[1] T. Martin, A. Crépieux, and N. Chtchelkatchev, Proceedings of NATO ARW on Quantum Noise in Mesoscopic Physics (Delft), edited by Yu. V. Nazarov and Ya. M. Blanter (May 2003, Kluwer Academic Publishers).
[2] A. Crépieux, R. Guyon, P. Devillard, and T. Martin, Phys. Rev. B 67, 205408 (2003).

### M1B2        **Electron-hole entanglement and teleportation**

C. W. J. Beenakker[1], C. Emary[1], M. Kindermann[1], J. L. van Velsen[1]
*1) Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands*

We demonstrate theoretically that the shot noise produced by a tunnel barrier in a two-channel conductor violates a Bell inequality. The non-locality is shown to originate from entangled electron-hole pairs created by tunnelling events — without requiring electron-electron interactions. Building on this scheme, we show how the annihilation of an electron and a hole by elastic scattering leads to teleportation of the (unknown) state of the annihilated electron to a second, distant electron — if the latter was previously entangled with the annihilated hole.

### M1B3        **Entanglement in Noninteracting Mesoscopic Structures.**

A. V. Lebedev[1], G. B. Lesovik[1], G. Blatter[2], C. W. J. Beenakker[3]
*1) L. D. Landau Institute for Theoretical Physics RAS, 117940, Russia*
*2) Theoretische Physik, ETH-Hönggerberg, CH-8093, Zürich, Switzerland*
*3) Instituut-Lorentz, Universiteit Leiden, P.O. Box 9506, 2300 RA Leiden, The Netherlands*

We study time dependent electron-electron and electron-hole correlations in mesoscopic devices splitting an incident current of free fermions into two spacially separated particle streams. We analyze the appearance of entanglement as manifested through a Bell inequality test and locate its origin either in the local spin-singlet correlations of the injected pairs or in a wave function projection during the Bell measurement, depending on the particular choice of the source of incident particles. The time window over which the Bell inequality is violated is determined in the tunneling limit and for the general situation with arbitrary transparencies.

M1B4     **Two-particle Aharonov-Bohm effect and entanglement in the electronic Hanbury Brown Twiss setup.**

Peter Samuelsson[1], Eugene Sukhorukov[1], Markus Buttiker[1]
*1) University of Geneva, Switzerland*

We analyze a Hanbury Brown Twiss geometry in which particles are injected from two independent sources into a mesoscopic electrical conductor in the quantum Hall regime. All partial waves end in different reservoirs without generating any single particle interference, however, exchange effects lead to two particle interference. We demonstrate that this effect is connected to orbital entanglement, electron-hole entanglement as well as post-selected electron-electron entanglelment. The entanglement is detected via a violation of a Bell Inequality, expressed in terms of zero frequency current correlators. The transport is along edge states and only adiabatic quantum point contacts and normal reservoirs are employed. A comparison to the optical Hanbury Brown Twiss effect is performed.

M1B5     **Entangled electrons from Coulomb scattering in a 2DEG**

D.S. Saraga[1], B.L. Altshuler[2], D. Loss[1], R.M. Westervelt[3]
*1) Department of Physics and Astronomy, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland*
*2) Physics Department, Princeton University, Princeton, NJ 08544*
*3) Division of Engineering and Applied Sciences, Harvard University, MA 02138*

We propose a setup to generate non-local spin-EPR pairs via pair collisions in a 2D interacting electron gas, based on constructive two-particle interference in the spin singlet channel at a $\pi/2$ scattering angle [1]. We calculate the scattering amplitude via the Bethe-Salpeter equation in the ladder approximation and small $r_s$ limit, and find that the Fermi sea leads to a substantial renormalization of the bare scattering process. From the scattering length we estimate the current of spin-entangeld electrons and show that it is within experimental reach.
[1] D.S. Saraga, B.L. Altshuler, Daniel Loss, R.M. Westervelt, Phys. Rev. Lett. (to be published); cond-mat/0310421.

M1B6     **Clauser-Horne inequality and entanglement in mesoscopic conductors**

Fabio Taddei[1], Lara Faoro[2], Rosario Fazio[1]
*1) NEST-INFM & Scuola Normale Superiore, Pisa, Italy*
*2) Department of Physics and Astronomy, Rutgers University, USA*

We derive a Clauser-Horne (CH) inequality for the full electron counting statistics in a mesoscopic multiterminal conductor and we discuss its properties. We first consider the idealized situation in which a flux of entangled electrons is generated by an entangler and sent into two spatially separated terminals, where the counting is performed. Given a certain number of incoming entangled electrons, the CH inequality can be evaluated for different numbers of transmitted particles. Strong violations occur when the number of transmitted charges on the two terminals is the same, whereas no violation is found for different numbers of transmitted particles. We then consider two actual setups: a hybrid superconducting structure, where two normal-metallic wires are connected to a superconductor, and a three terminal normal beam splitter.

*Physics of f-electron materials I. (PCFES 7)* **Room C**

M1C1 **Photoemission Study at the *5f* Localization Threshold - Pu and Am: Metal, Nitride and Hydride**

T. Gouder[1], P. M. Oppeneer[2], F. Wastin[1], J. Rebizant[1]
*1) European Commission, Joint Research Centre, Institute for Transuranium Elements, Postfach 2340, D-76125 Karlsruhe, Germany*
*2) Leibniz-Institute of Solid State and Materials Research, P.O. Box 270016, D-01171 Dresden, Germany*

Pu and Am are located at the *5f* localization-delocalization threshold. One important question is, whether the photoemission spectra of Pu still reflect the ground-state DOS or whether they contain already final state features (multiplets and correlation satellites).

We compare photoemission spectra of metal, nitrides and hydrides, presenting different degrees of *5f*-hybridization. Am always has well localized *5f* states in a *5f*$^6$ configuration. Pu systems are more complex. Spectral features show the coexistence of band like ($\alpha$-Pu), and two localized configurations (*5f*$^5$ and *5f*$^6$) which appear as characteristic multiplet structures in the photoemission spectra.

M1C2 **Actinides, Superconductivity and Mott transition : the case of Americium**

J.-C. GRIVEAU[1], J. REBIZANT[1], G.H. LANDER[1], G. KOTLIAR[2]
*1) European Commission, Joint Research Centre, Institute for Transuranium Elements, Postfach 2340, 76125 Karlsruhe, Germany*
*2) Center for Materials Theory, Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA*

With electronic ground state J=0 (no magnetic moment), americium presents 5f electrons localized. We report high-pressure measurements of the resistivity of dhcp americium metal up to 27 GPa and down to 400 mK. The unusual dependence of the superconducting temperature ($T_c$) on pressure is deduced. The critical field increases dramatically from 0.05 to $\sim$ 1 T in Am I phase as the pressure is increased, suggesting a change from type I to type II superconductor. At a highest pressure (Am II - Am III), the 5f electrons of Am are changing from localized to itinerant, with a change of the crystal structure. The role of a Mott-type transition in this development of superconductivity is postulated.

M1C3 **The condensed-matter physics of Plutonium; a "heavy-fermion" element**

John Singleton[1], John Betts[1], Paul Goddard[1], Jason Lashley[1], Ross McDonald[1], Charles Mielke[1], Albert Migliori[1]
*1) National High Magnetic Field Laboratory, TA-35, MS-E536, Los Alamos, NM87545, USA*

Plutonium is perhaps the most interesting element in the Periodic Table; it represents the boundary between localised (Am) and delocalised (Np) $5f$ electrons in the Actinide series. The resultant small energy scales, large density of states and general instability of the $5f$-electron system are probably the cause of many of Pu's extraordinary properties, including its six distinct solid phases at ambient pressure. I shall describe recent heat-capacity, magnetization, skin-depth and magnetoresistance experiments on $\alpha$ and $\delta$ Pu at the National High Magnetic Field Laboratory. The data give important clues about the energy scales and behaviour of the $f$ electrons.

M1C4 **Delocalization vs. Spin-Orbit Splitting in the Actinide 5f States**

JG Tobin[1], KT Moore[1], BW Chung[1], MA Wall[1], AJ Schwartz[1], G van der Laan[2]
*1) Lawrence Livermore National Laboratory, Livermore, California 94550, USA*
*2) Synchrotron Radiation Source, Daresbury Laboratory, Warrington, WA4 4AD, UK*

The Spin-orbit moment can be used as a measure of the degree of localization of valence electrons in a material. Here, we measure the degree of 5f localization in the light actinide metals, Th, U, and Pu, using the branching ratio of the white line peaks of the N4,5 edges acquired by electron energy-loss spectroscopy in a transmission electron microscope, synchrotron-radiation-based X-ray absorption, and multi-electronic atomic spectral simulations. Examination of the branching ratios shows that the apparent spin-orbit splitting is partially quenched in alpha-U, but is strongly dominant alpha-Pu. These results are fully quantified using the sum rule. This work was performed under the auspices of the U. S. Department of Energy by the University of California, Lawrence Livermore National Laboratory under Contract No. W-7405-Eng-48.

*P-wave pairing in metals* **Room D**

M1D1 **Realistic gap models for superconducting Sr2RuO4**

J F Annett[1], G Litak[2], K I Wysokinski[3], B L Gyorffy[1]
*1) HH Wills Physics Laboratory, University of Bristol, Tyndall Avenue, Bristol, BS8 1TL, UK*
*2) Department of Mechanics, Technical University of Lublin, Nadbystrzycka 36, 20-618 Lublin, Poland*
*3) Institute of Physics, M. Curie Sklodowska University, Radziszewskiego 10, 20-031 Lublin, Poland*

$Sr_2RuO_4$ is believed to be a spin triplet Cooper paired system. However the nature of the gap on the Fermi surface is controversial because the pairing state must have both chiral symmetry and line nodes on the Fermi surface. We have proposed a gap model in which horizontal lines of nodes are present because of interplanar coupling between Ru $d_{xz}$ and $d_{yz}$ obitals. We shall review the current state of the theory and the experimental situation. We shall also present new results on the effects of spin-orbit coupling and magnetic fields on this pairing state.

M1D2 **P-wave pairing correlations in S-F hybrid structures**

Matthias Eschrig[1]
*1) Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany*

P-wave pairing correlations are important in s-wave superconductor-ferromagnet heterostructures with a mean free path comparable to or larger than the superconducting coherence length. In the case of a strong ferromagnet sandwiched between two s-wave superconductors, they dominate the Josephsoneffekt through the ferromagnet. In this case, p-wave pairing correlations stabilize $\pi$-Josephson junctions. The mechanism is due to the creation of mixed parity states in superconducting regions close to an interface with a strong ferromagnet. We discuss situations for which such p-wave correlations in heterostructures containing strong ferromagnets lead to new physics in comparision to heterostructures with weak ferromagnets.

M1D4 **Electronic theory for normal-state spin dynamics in $Sr_2RuO_4$**

Dirk Manske[1], Ilya Eremin[2], Karl Bennemann[2]
*1) Max-Plank Institut for Solid State Research, Stuttgart, Germany*
*2) Institute for Theoretical Physics, Free University of Berlin, Berlin, Germany*

The novel spin-triplet superconductivity with $T_c = 1.5K$ observed in layered $Sr_2RuO_4$ seems to be a new example of unconventional superconductivity. Using the three-band Hubbard Hamiltonian we calculate the spin susceptibility, $\chi(\mathbf{q}, \omega)$, and the NMR spin-lattice relaxation rate, $1/T_1$, in the normal state within the random-phase-approximation and find quantitative agreement with experimental data. Most importantly, at low temperatures, we find that the out-of-plane component of the spin susceptibility, $\chi^{zz}$, becomes almost two times larger than the in-plane one, $\chi^{+-}$, due to spin-orbit coupling. These results support a scenario of Cooper-pairing mediated by spin-fluctuations as the most probable mechanism to explain triplet superconductivity in $Sr_2RuO_4$. Finally, we discuss also the possibility of nodes occurring in the superconducting order parameter as proposed by several experimental interpretations and phenomenological theories.

M1E1    **Monte Carlo Simulations of Polylelectrolyte Multilayering**

René Messina [1]

*1) Institut für Theoretische Physik II, Heinrich-Heine-Universität Düsseldorf, Universitätsstrasse 1, D-40225 Düsseldorf - Germany*

The adsorption of highly and oppositely charged flexible polyelectrolytes (PEs) onto charged substrates is investigated by means of Monte Carlo simulations. A detailed study of the equilibrium structure of the first few PE layers is provided for three substrate geometries: (i) spherical, (ii) planar and (iii) cylindrical. The influence of the chain length and of a (extra) non-electrostatic short range attraction between the polycations and the negatively charged substrate is considered. It is shown that the stability as well as the microstructure of the PE layers are especially sensitive to the strength of this latter interaction. Besides, it is found that the formation of PE multilayers is also dependent on the substrate geometry. In particular, for the case of a thin cylindrical substrate, we demonstrate that the building up of PE multilayers is strongly prohibited mainly due to the high chain-entropy penalty stemming from the low dimensionality of the substrate.

M1E2    **Smart polyelectrolyte capsules as microcontainers and reactors**

Helmuth Moehwald[1]

*1) Max-Planck-Institute of Colloids and Interfaces, Research Campus Golm, 14424 Potsdam, Germany*

In recent years there has been much progress in the development and characterization of ultrathin polymeric films, and this knowledge could be transferred to coat colloids. This on one hand yielded systems with high specific surface area on the other hand removal of the colloidal template yielded micro-and nanocapsules with well-defined geometry, wall thickness and composition. Choosing suitable polymeric building blocks and modes of preparation one then can tune the permeability and mechanical properties. One thus obtains smart containers which on one hand are promising for drug encapsulation and release on the other hand they are interesting microreactors with selective permeation for educt or/and product lending encapsulated catalysts an optimized environment.

M1E3    **Polyelectrolyte Brushes as substrates for polyelectrolyte mulitlayers**

Jurgen Ruhe[1], Haining Zhang[1], Duan-Cong Vo[1], Rupert Konradi[1]
*1) Institute for Microsystems Technology, University of Freiburg, Germany*

Polyelectrolyte brushes are interesting substrates for the formation of monolayers of polyelectrolyte-polyelectrolyte complexes and for the deposition of polyelecrolyte multilayers in a layer-by-layer deposition procedure. We describe the results of recent experiments on the interaction of surface-attached monolayers of weak polyelectrolytes with low molecular weights salts in a contacting environment and on the interaction of the brush monolayers with polyelectrolyte molecules in solution. The influence of layer thickness, graft density of the brush, pH-value and salt concentration of the solution and other parameteres will be elucidated. A comparison between the behavior of weak and strong surface-attached polyelectrolyte complexes will be made.

M1E4 **From Functional Core/Shell Nanoparticles to Empty Nanospheres**

Gregory Schneider[1]

*1) Institute Charles Sadron (CNRS), 6 rue Boussingault, F-67083 Strasbourg-Cedex, France and University Louis Pasteur, 1 rue Blaise Pascal, F-67008 Strasbourg-Cedex, France.*

The adsorption (wrapping) of polyelectrolytes onto (around) oppositely charged nanospheres is a problem in colloid science (stabilisation, surface functionalisation), biology (DNA-histone complex) and in theoretical physics. Here we report that gold nanoparticles can easily be coated using LbL deposition as the sole method. The resulting core/shell nanoparticles are so well stabilised that they can be centrifuged and re-dispersed without agitation or use of ultrasound. At an average recovery of about 95 per cent of particles per layer, at least 20 layers can be deposited with a minimum of particle aggregation. Thus LbL opens a new and general route for the functionalisation of nanoparticles even in aqueous media limiting the risk of ligand exchange reactions. In the case of gold colloids, the core can be gently dissolved resulting in empty nanospheres.

M1E5 **Mechanical properties of polyelectrolyte multilayer microcapsules studied by atomic force and confocal microscopy.**

Olga I. Vinogradova[1]

*1) Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany*

We have suggested a novel approach to probe mechanical properties of "hollow" and "filled" multilayer microcapsules based on combination of atomic force and confocal microscopy. This talk will focus on new opportunities provided by our method: (i) simultaneous measurements of the capsule shape during the compression, (ii) a possibility to work with very small capsules, and (iii) monitoring the capsule volume, shell permeability for small and large molecules, and redistribution of the inner polymer at different stage of deformation. A discussion of main experimental observations and results (Young's modulus of the multilayer shells, effect of pH, salt, organic solvent, inner polymer etc on the capsule stiffness) will also be given.

*High pressure phenomena in physics* **Room F**

## M1F1    High-Pressure Physics in Material Science. Jahn-Teller systems.

Fernando Rodriguez[1]
*1) DCITIMAC, Facultad de Ciencias, Universidad de Cantabria, 39005, Santander, Spain*

There is an ever increasing activity in High-Pressure (HP) research as a consequence of the development of HP techniques. It has led to many scientific and technological areas to progressively incorporate HP techniques as an essential tool in their research. Nowadays the wide variety of topics in HP research demands more techniques and multidisciplinary activities and, in this context, physics plays a relevant role. An analysis of current topics of interest in materials science will be briefly presented along with open questions still deserving elucidation through HP techniques. The main emphasis will be on the pressure behaviour of certain materials incorporating transition metal ions either as a constituent or an impurity. In particular, the study of materials whose properties are related to Jahn-Teller ions will be commented on and discussed. Interestingly, the structural characterization of JT impurities, in some cases, facilitates the understanding the bulk properties of concentrated and pure materials. However, extracting structural information on these systems can be difficult and relies on the ability to establish structural correlations. We will explore alternative methods based on optical spectroscopy for the local structural characterization of JT ions in HP experiments. Recent results on layer perovskites of Mn3+ (AMnF4; A: Na, Tl, Cs) will be presented as an example.

## M1F2    Magnetoresistance of nanoscale magnets under high pressure

Gendo Oomi[1], Shiori Kaji[1], Yoshiya Uwatoko[2], Seiji Mitani[3], Koki Takanashi[3]
*1) Department of Physics,Kyushu University, Ropponmatsu, Fukuoka 810-8560, Japan*
*2) ISSP, University of Tokyo, Kashiwa 277-8581, Japan*
*3) IMR, Tohoku University, Sendai 980-8577, Japan*

The magnetoresistances (MR) of Co-Al-O films and Fe/Cr magnetic multilayers have been measured at high pressure and at low temperature. It is found that the MR of Co-Al-O is enhanced by applying pressure but the MR of $[Fe(20\text{\AA})/Cr(10\text{\AA})]_{20}$ decreases with increasing pressure. The enhancement of MR in Co-Al-O is attributed to the enhancement of the higher order tunneling effect. The decrease in the magnitude of MR in Fe/Cr magnetic multilayers is due to the suppression of the spin dependent resistivity by applying pressure. The saturation field increases with pressure, which is due to the increases in the magnitude of interlayer exchange coupling. Recent results for other systems will be reported briefly.

## M1F3    Electric conductivity studies at megabar pressures

Mikhail Eremets[1]
*1) Max Planck Inst. fr Chemie, Postfach 3060, 55020 Mainz, Germany*

Electrical measurements provide indisputable proof of the existence of a metal or non-metal, but present an experimental challenge at megabar pressures. We developed measurements up pressures of 260 GPa. We found that boron transforms to a superconductor near 160 GPa. We found superconductivity in Lithium - the lightest and the simplest metal. Tc ranges from 9 to 16 K at 23 to 80 GPa that is much lower than those predicted theoretically. Nitrogen represents a unique way of transformation - to a polymeric structure in which each atom is bonded to three nearest neighbours by single covalent bonds. It is a semiconductor with energy gap of 0.4 eV at 240 GPa. We performed the first attempt of direct measurements of conductivity of hydrogen at pressures up to 250 GPa it remains insulator. We will also present new developments on achievement and measurements of the highest static pressures.

M1F4    **<u>Group IVa Hydrides at High Pressure: High Temperature
Superconductors?</u>**

A. Bergara[1], N.W. Ashcroft[2]

*1) Condensed Matter Physics Department, University of the Basque Country, and DIPC*
*2) Laboratory of Atomic and Solid State Physics, Cornell University*

*Simple* elements (e.g. alkalis) show an interesting *complex* behaviour under high pressure. For example, recent experiments have shown that lithium superconducts at 15 K when the applied pressure rises to around 30 GPa. This interesting observation has renewed the interest of hydrogen as a possible candidate to superconduct at room temperature, however, the required metallization cannot be reached experimentally yet. In this talk we propose the group IVa hydrides, where hydrogen is the dominant constituent, as new candidates as high temperature superconductors. These hydrogen dominant alloys share similar arguments than pure metallic hydrogen to become superconductors but pressures considerably lower might be necessary to attain the required metallic states.

*Mechanical properties of metallic glasses* **Room G**

## M1G1    BULK METALLIC GLASSES - GLASS FORMABILITY AND FLOW

H.A. Davies[1], I. Todd[1]
*1) Dept. Engineering Materials, Univ. of Sheffield, Sheffield S1 3JD, U.K.*

The discovery and evolution over the past decade of several new families of metallic alloy compositions which can be fully vitrified in thick sections has refocussed attention on the factors that influence glass forming ability, GFA, of alloys. The reduced glass temperature, RGT, proved to be a useful figure of merit for predicting GFA for the more conventional metallic glass formers. However, the usefulness of the RGT for bulk glass formers is more problematical. The various reasons for this will be discussed. The discussion will encompass the viscous flow characteristics of bulk glass forming alloys, for which data exist, and, in particular, a comparison with the behaviour of alloys of low and intermediate glass forming abilities, to examine the degree to which any clear differences in behaviour exist between them. The validity of other parameters for correlating with GFA will also be considered.

## M1G2    Microstructure design for strengthening of metallic glasses

J. Eckert[1]
*1) TU Darmstadt, FB 11 Material- und Geowissenschaften, FG Physikalische Metallkunde, Petersenstr. 23, D-64287 Darmstadt, Germany*

Metallic glasses offer high strength, but usually lack macroscopic ductility. An additional phase is needed for toughening. Hence, it is of strong interest to develop a one-step process that can directly produce structural metallic glasses, e.g. through casting, with an in situ formed composite microstructure that combines phases with different desirable properties. This can be realized in primary-dendrite-glassy/nanostructured matrix composites, where a strong matrix is combined with ductile beta-Ti-type dendrites as the toughening phase. Results of the structural and compositional analysis of the microstructures of such composites will be presented. The phase formation will be described considering the solidification parameters and the conditions required to form the composite. The microstructure will be correlated with the mechanical properties to demonstrate the desirable high strength and plasticity that can be obtained for such composites.

## M1G3    Mechanisms of diffusion and viscous flow in bulk glass-forming alloys

F. Faupel[1], V. Zöllmer[1], A. Bartsch[1], K. Rätzke[1]
*1) Kiel University, Chair for Multicomponent Materials, Kaiserstr. 2, 24143 Kiel, Germany*

We review radiotracer diffusion and isotope effect measurements in metallic bulk glass-forming alloys from the glassy state to the equilibrium melt and compare diffusion and viscous flow [1]. In the glassy as well as in the deeply supercooled state below the critical temperature $T_c$ the very small isotope effects indicate a highly collective hopping mechanism. In the supercooled state below $T_c$ the temperature dependence is Arrhenius-type with an effective activation enthalpy, and diffusion is decoupled from viscosity. Above $T_c$ the onset of liquid-like motion is evidenced by a gradual drop of the effective activation energy and by the validity of the Stokes-Einstein equation. This strongly supports the mode coupling scenario. The isotope effect measurements show atomic transport up to the equilibrium melt to be far away from the regime of uncorrelated binary collisions.
[1] F. Faupel, et al. Rev. Mod. Phys. 75 (2003) 237.

M1G5　**Mechanical response in bulk metallic glasses: elastic, viscoelastic and viscoplastic components. Influence of a nanocrystallization.**

J.M. PELLETIER[1]

*1) GEMPPM, Bat. B. Pascal, INSA-Lyon, 69621 Villeurbanne Cedex, France*

The dynamic mechanical response was investigated in bulk metallic glasses in large temperature and frequency ranges. Mechanical spectroscopy was performed either using continuous heating or isothermal measurements, but in any case only limited deformations are involved. A main viscoelastic relaxation is observed before the onset of crystallization. The very large values of activation energy and pre-exponential factor indicate that this relaxation involves the collective movement of a large number of atoms, as in many amorphous materials (polymers, oxide or molecular glasses). Master curves are plotted, indicating that the time-temperature superposition principle is obeyed. These master curves can be described using a physical model based on the concept of quasi-point defects. The elastic, viscoelastic and viscoplastic contributions to the deformation are separated. Finally, the influence of a nanocrystallization is investigated.

*Theory of optical and dielectric properties in condensed matter* **Room H**

M1H1 **Quasiexcitons and bound excitons in extended systems: Many–Body versus time–dependent density–functional approach**

Andrea Marini[1], Rodolfo Del Sole[2], Angel Rubio[1]
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*2) INFM e Dipartimento di Fisica dell'Università "TorVergata", I–00133 Roma, Italy*

Excitons are ubiquitous in our understanding of the optics of extended systems. Their first principle description is achieved by solving the Bethe–Salpeter equation (BSE) of Many–Body Perturbation Theory. We discuss the solution of the BSE in presence of a time–dependent electron–hole interaction that, in contrast to common belief, implies non negligible excitonic effects in the optical spectra of metals.

An alternative approach to the BSE is Time–Dependent–Density–Functional Theory, where all many-body effects are cast into the exchange–correlation kernel $f_{xc}$. We present a BSE–based derivation of a frequency dependent and non–local $f_{xc}$ that correctly describes strongly and weakly correlated excitons, as we show in the case of LiF, $SiO_2$ and diamond.

M1H2 **Parameter-free calculation of response functions in time-dependent density-functional theory**

Francesco Sottile[1], Valerio Olevano[1], Lucia Reining[1]
*1) Laboratoire des Solides Irradiés, École Polytechnique, F-91128 Palaiseau, France*

We have established and implemented a fully *ab initio* method which allows one to calculate optical absorption spectra of semiconductors and insulators, including excitonic effects, without solving the cumbersome Bethe-Salpeter equation, but obtaining results of the same precision. This breakthrough has been achieved in the framework of time-dependent density-functional theory, using new exchange-correlation kernels $f_{xc}$ that are free of any empirical parameter. We show that the same excitonic effects in the optical spectra can be reproduced through different $f_{xc}$'s, ranging from frequency-dependent ones to a static one, by varying the kernel's spatial degrees of freedom. This indicates that the key quantity is not $f_{xc}$, but $f_{xc}$ combined with a response function. We present results for the optical absorption of bulk Si, SiC (exhibiting continuum exciton effects) and bulk Argon (exhibiting instead a bound exciton series) in good agreement with experiment, almost indistinguishable from those of the Bethe-Salpeter approach.

M1H3 **Time-dependent spin-current-density functional theory**

Giovanni Vignale[1]
*1) University of Missouri-Columbia*

Ordinary time-dependent density functional generally suffers from an ultra-nonlocality problem, namely the local density approximation for the exchange-correlation potential always fails, no matter how slowly varying the density is. This problem is particularly severe in time-dependent spin-density functional theory, but can be cured by switching to a formulation in which the spin currents are the basic variables. I discuss the physical significance of the new terms that appear in the spin-current dependent functional, and review the progress that has been made in providing explicit expressions for the latter.

M1H4    **Conserving theories for the Response Functions of Time-Dependent Density-Functional Theory.**

Ulf von Barth[1]
*1) Dept. of Physics, Lund University*

It is rather well known that the optical or density response function of electronic systems can be obtained from time-dependent density-functional theory (TDDFT) in terms of an exchange-correlation kernel (fxc). This approach is computationally far simpler as compared to solving the Bethe-Salpeter equation of many-body perturbation theory (MBPT). Unfortunately, within TDDFT, no systematic route toward successively better approximations has, so far, been available. In the present work we construct such a scheme based on our variational action functionals having the one-electron Green function of MBPT as their basic variable. By restricting the variational freedom of the functionals to Green functions which are non-interacting and given by a local one-electron potential, we automatically obtain a TDDFT and an fxc corresponding to every choice of variational functional. Functionals based on PHI derivable theories give particle conserving fxc:s.

*Mesoscopics* **Room J**

## M1J1  Magnetic-field asymmetries in nonlinear mesoscopic transport

David Sanchez[1]
*1) University of Geneva*

The Onsager relations applied to electronic transport state that the conductance of a two-terminal conductor is an even function of the magnetic field. However, breakings of this symmetry may take place in the nonlinear regime. We find that magnetic-field asymmetries indeed arise in mesoscopic systems out of equilibrium but, interestingly, only as a consequence of the charge response of the conductor, thus being a pure interaction effect [1]. We illustrate this result for two types of conductors: a quantum Hall bar with an antidot and a ballistic chaotic cavity connected to quantum point contacts. For the latter, we obtain through random matrix theory an asymmetry in the fluctuations of the nonlinear conductance. A metallic diffusive cavity has been recently treated [2] whereas experiments are currently in progress [3].

[1] D. Sanchez and M. Buttiker, condmat/0404387 (unpublished). [2] B. Spivak and A. Zyuzin, cond-mat/0404408 (unpublished). [3] D.M. Zumbuhl et al., unpublished (2004).

## M1J2  Mesoscopic mechanical systems

A. D. Armour[1]
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Recent developments in fabrication have made it possible to produce nanoelectromechanical systems in which mechanical resonators with frequencies up to 1 GHz are coupled electrostatically to mesoscopic conductors. The mechanical degrees of freedom in nanoelectromechanical systems can be thought of as mesoscopic in the sense that when cooled to ultra-low temperatures, they are expected to display a crossover from classical to quantum behaviour under certain circumstances. We describe the dynamics of a nanomechanical resonator coupled to two different types of electronic system: a single electron transistor and a Cooper-pair box. When a resonator is coupled to a single electron transistor, the transport electrons act on the resonator almost exactly like a thermal bath and its motion can in general be described classically. In contrast, when a resonator is coupled to a Cooper-pair box it can be driven into a superposition of spatially separated states and therefore must be described using quantum mechanics.

## M1J3  Current noise in nanoelectromechanical systems

T. Novotný *[1], A. Donarini[1], C. Flindt[1], A.-P. Jauho[1]
*1) MIC - Department of Micro and Nanotechnology, Technical University of Denmark*

Nanoelectromechanical systems (NEMS) are presently a topic of intense research activity. These devices combine electronic and mechanical degrees of freedom to display new physical phenomena, and potentially may lead to new functionalities. Therefore, the electronic transport in these systems has been studied recently theoretically as well as experimentally. Since the mean current alone may not provide enough information to distinguish between different electronic transport mechanisms within NEMS the current noise spectrum is a natural choice to consider in order to characterize the device better. We present a theory of the current noise in NEMS which can be described by Markovian generalized master equations and apply it to various systems — single dot quantum and classical shuttles and a vibrating quantum dot array. We evaluate the noise spectrum numerically, discuss some of its characteristic features in the different cases, and compare them with semi-analytical predictions based on physically motivated approximate treatments. * also at Department of Electronic Structures, Charles University, Prague

M1J4    **Electron-vibron coupling in molecular transistors**

Karsten Flensberg[1]
*1) Niels Bohr Institute*

The talk discusses electromechanical effects in molecular transistor. First, broadening of Franck-Condon sidebands is analyzed in terms of both the life-time of the vibrational modes and of the electronic levels. Second, recent results on correlation effects in molecular transistors are discussed.

# Poster Session 16:00 – 18:00

S1X1 **High Frequency Properties of Nanometer Semiconductor Structures**

Michal Horak[1]

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Potential barriers of different types and quantum wells are substantial parts of a wide spectrum of micro- and nanoelectronic devices. Depending on a layer composition, materials, doping profiles and external electric field electrons and holes in such structures participate in different emission and tunneling processes; thus quantum physics methods, especially the time dependent Schrdinger equation, should be used to describe these phenomena. Typical situation in electronics is that a dc-bias together with a small ac-signal are applied to the structure. The following results are presented in this paper: analytical formulae for the ac barrier transmittance (convenient for compact device models), the transmission amplitudes as functions of electron energy and the position of resonance peaks (the influence of dc bias, of different electron effective mass inside the barrier region etc.), complex admittance of the structure, one-dimensional high-frequency model of the nanoscale MOSFET transistor.

S1X2 **Coherent transport and electron-vibration coupling in molecular wires**

H. NESS[1]

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Molecular wires are subject to intense experimental and theoretical research. It is important to know their transport properties to assess their potential as molecular scale electron devices. In such systems, electron coupling to other excitations (phonons for instance) is expected to govern the transport properties. We calculate the transport through molecular junctions taking into account the coupling of the electron with quantum phonons in the molecule. The propagation of a tunneling electron through "long" molecules induces atomic displacements corresponding to the formation of a polaron. The polaron can interact strongly with a pre-exisiting soliton in the molecule. The coherent quantum electron-phonon interactions strongly modify the transmission through the wires. For short wires, phonon side-band peaks appear around molecular resonances. The presence of such peaks can explain the behaviour of the resonances' widths with temperature.

S1X3 **Spin coherence dynamics in CdS nanocrystals at room temperature**

P. Nemec[1], D. Sprinzl[1], P. Nahalkova[1], F. Trojanek[1], P. Maly[1]

*1) Charles University in Prague, Faculty of Mathematics and Physics, Ke Karlovu 3, 121 16 Prague 2, Czech Republic*

Recently, the increase of spin-relaxation time in quantum dots as compared to the bulk and quantum well samples was proposed. In this paper, we report on the room temperature spin relaxation measurements in CdS nanocrystals in glass matrix. We investigated the spin relaxation of the electrons by performing ultrafast laser polarization-resolved pump-probe experiments in nanocrystals with radius of 2.5 nm. We found that the photoexcited population of carriers decay strongly nonexponentially with the effective lifetime (decay to 1/e) of about 90 ps. On the contrary, we observed that the spin-relaxation time is extremely long - reaching at least 10 ns. So, it means that even at room temperature basically all electrons throughout their lifetime maintain the original spin-polarization. This shows that semiconductor nanocrystals are a very promising material for spintronics and quantum computation where the long spin-relaxation time is essential.

S1X4 **High-order current correlation functions in the Kondo systems.**

A. Golub[1]

*1) Department of Physics, Ben-Gurion University, Israel.*

For additional information which helps to distinguish between stochastic processes we need to compute high-order cumulants. Here we examine the statistics of current fluctuations in junctions with quantum dots. We consider strongly interacting limit when the dot is in the Kondo regime. With the help of modified Keldish technique we, unlike the recent computations for interacting systems, for the first time directly calculate the symmetric (non ordering in time) three currents correlation function or third current cumulant. As a function of ratio v=eV/Tk 3rd cumulant was obtained for tree different regimes: Fermi liquid regime (v¡1), crossover interval (v 1) and RG limit (v¿¿1). Correspondingly, several approximation schemes have been applied: mean field slave boson theory, NCA, renormalization group calculations. Unlike the case of noninteracting dot, in the Kondo regime 3rd cumulant shows strong non-linear voltage dependence. Only in the asymptotical limit of large voltages the linear dependence on V is restored.

S1X5 **NI-SQUID: Normal metal - Insulator - Superconductor Quantum Interference Device**

K. Yu. Arutyunov[1], T. T. Hongisto[1]

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Hybrid normal metal - insulator - superconductor microstructures suitable for studying an interference of electrons were fabricated. The structures consist of a superconducting loop connected to a normal metal electrode through a tunnel barrier. All measurements were performed at temperatures well below 1 K. The interference can be observed as periodic oscillations of the tunnel current (voltage) through the junction at fixed bias voltage (current) as a function of a perpendicular magnetic field. The magnitude of the oscillations depends on the bias voltage V. It reaches a maximum at energy eV which is close to the superconducting gap and decreases with an increase of temperature. Surprisingly, the period of the oscillations in units of magnetic flux is equal neither to h/e nor to h/2e, but significantly exceeds these values for larger loop circumferences. Possible explanations of the phenomena are discussed.

S1X6 **Current Noise of Shuttle Devices**

A. Donarini[1], T. Novotný *[1], C. Flindt[1], A.-P. Jauho[1]

*1) MIC – Department of Micro- and Nanotechnology, Technical University of Denmark*

Current noise calculation is presented for an archetypical shuttle device consisting of a movable quantum dot confined by a parabolic potential and electrically connected to leads. Changing mechanical damping we bring the system from (renormalized) resonant tunneling to shuttling regime in which the oscillating dot transfers one electron per cycle. The zero-frequency noise measured by the Fano factor F reaches very low values ($F \approx 0.01$) in the shuttling regime even in the quantum limit, confirming that shuttling is universally a low noise phenomenon. In approaching the semiclassical limit, the Fano factor shows a giant enhancement ($F \approx 100$) at the shuttling threshold, consistent with predictions based on phase-space representations of the density matrix. We also model the charge transport through the system at the shuttling threshold as a slow dichotomous process between the resonant tunneling and the shuttling current channels. Based on this model an independent calculation of the Fano factor is performed. * also at Department of Electronic Structures, Charles University, Prague

S1X7 **Overlaping of vertically stacked quantum dot electron wavefunctions**

A. Hospodkova[1], K. Kuldova[1], J. Oswald[1], E. Hulicius[1], J. Pangrac[1], I. Vavra[2]
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*2) Inst. of El. Eng., SAS, Dubravska cesta, Bratislava, 842 39, Slovak Republic*

A possible way to increase the InAs/GaAs quantum dot (QD) emission wavelength up to $1.3\,\mu$m (optical communication) is to increase the QD size in vertically stacked QD structures. We have grown these strustures with different thickness of spacers between QD layers. The increase of QD size from the 1st to the 7th grown QD layer is evident from the TEM image of our stacked QDs. Photo- and magnetophotoluminescence measurements were used for sample characterization. We have studied the overlap of electron wavefunctions of stacked QDs. We have found that for spacer thickness around 7 nm electron wave functions of smaller stacked QDs in the deeper layers still overlap while the electron wave functions of bigger QDs in the top layers remain separated. For thicker spacers all wavefunctions seem to be spatially separated.

S1X8 **Ferromagnetic magnetic-dipolar-mode quantum dots**

Eugene Kamenetskii[1], Reuven Shavit[1], Michael Sigalov[1]
*1) Department of Electrical and Computer Engineering, Ben Gurion University of the Negev, Israel*

In a case of magnetic dipolar modes (MDM) in a normally magnetized ferrite disk one can formulate the energy eigenvalue problem for the magnetostatic wave function. MDM spectra in a normally magnetized thin-film ferromagnetic disk have discrete energy eigenstates and can be described as a collective motion of quasiparticles, the light magnons [1]. The properties elucidate the macroscopic quantum confinement effect in disk-form ferrite dots. To a certain extent this resembles study of the eigenvalue problem for the Schroedinger operator on a two dimensional semiconductor disk. We give an analysis of the fields and states in a disk-shaped ferromagnetic MDM quantum dots. To take into account the internal DC field inhomogeneity preserving, at the same time, the quantized "spectral portrait" of MDM oscillations, we use the method of the Green functions. [1] E.O. Kamenetskii, R. Shavit, and M. Sigalov, Europhys. Lett., 64, 730 (2003).

S1X9 **Anapole moments in MS-wave ferrite disks**

Eugene Kamenetskii[1]
*1) Department of Electrical and Computer Engineering, Ben Gurion University of the Negev, Israel*

The anapole moments take place in systems with the parity violation and with the annual magnetic field. The anapole-moment properties are important in condensed matter physics. The notion of the anapole was used for explanation of the magnetoelectric (ME) effect in solid-state magnetic crystals and should underlie the physics of the microwave ME effect in thin-film ferrite disks. MS-wave oscillations in ferrite samples occupy a special place between the pure electromagnetic and spin-wave (exchange) processes. These microscopic oscillating objects the particles may interact with the external EM fields by a very specific way, forbidden for the classical description. The presence of surface magnetic currents is one of the features of MS oscillations in a normally magnetized ferrite disk. Because of such magnetic currents, MS oscillations in ferrite disk resonators become parity violating [1]. [1] E.O. Kamenetskii, Europhys. Lett, 65, 269 (2004).

S1X10 **Quantum interference of electrons in $Nb_5Te_4$**

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*2) Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany*

The quasi-one-dimensional compound $Nb_5Te_4$ undergoes a transition to superconductivity at $\sim$0.8 K. Its electronic transport properties in the normal state are studied as a function of temperature and magnetic fields up to 12 T. The temperature variation of the resistivity is weak ($\leq$3% in the range 1.2–300 K) and a nonmonotonic behaviour is observed which is characterized by two local maxima at $\sim$2 K and $\sim$30 K. Both the temperature dependence of the resistivity and the magnetoresistance are analyzed and interpreted as due to an interplay of weak localization, weak antilocalization, and electron-electron interaction effects in the diffusion and the Cooper channels. The nearly linear temperature dependence of the resistivity observed towards higher temperatures is ascribed to non-Fermi-liquid behaviour of charge carriers.

S1X11 **Current noise in a vibrating quantum dot array**

C. Flindt[1], T. Novotný *[1], A. Donarini[1], A.-P. Jauho[1]
*1) MIC - Department of Micro and Nanotechnology, Technical University of Denmark*

We study electron transport through a triple-dot array in the strong Coulomb blockade regime. The central dot can vibrate mechanically, leading to a complicated interplay between electron transport and mechanical motion. Based on two different approaches, the quantum regression theorem and full counting statistics, we derive expressions for the zero-frequency current noise, and we show that the two approaches are equivalent. The current noise is evaluated numerically, and depending on the model parameters we identify co-tunnelling between the outer dots, shuttling via the central dot, or sequential tunnelling between neighboring dots as the leading mechanism of transport. In the limit of weak inter-dot coupling we derive analytic expressions for the current noise, which validate the sequential tunnelling interpretation of the numerical results. * also at Department of Electronic Structures, Charles University, Prague

S1X12 **Directional scattering in two dimensional electron gas**

Ismet I. Kaya[1]
*1) Faculty of Engineering and Natural Sciences, Sabanci University, İstanbul 34956, Turkey*

Directional scattering of electrons is observed in GaAs/AlGaAs two dimensional electron gas. A cross junction with electrostatic emitter and collector barriers on two opposite terminals has been patterned on a high mobility 2DEG structure. In the transition from the linear ballistic transport regime as electron energies are increased, single or few e-e scattering events dominate the transport properties of the device. This is distinctive, unlike linear ballistic or diffusive transport, in which the inter-carrier scattering is either almost completely eliminated or abundant. Our results show that in this regime directionality is still preserved after momentum transfer between the electrons over distances longer than 5 $\mu$m. It has been observed that with an asymmetrical device geometry and tuned energy barriers, directional scattering reverses the current in the crossing terminals and yields negative resistance.

S1X13 **Electron and Optical Properties of Two-Dimensional and Three-Dimensional Quantum Dots in Magnetic Field**

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*2) Institute of Spectroscopy, Academy of Sciences of Russia, 142190 Troitsk, Russia*

We investigate theoretically 2D and 3D quantum dots (QD). We calculated energy and wave function spectra, which determine electron and optical properties of QD. Influence of Coulomb interaction between electrons and magnetic field is considered. We have studied single QD and QD systems (horizontally and vertically coupled) analytically and numerically. Strong correlation effects are analyzed. Electron crystallization and short-order appearance are studied. Strong magnetic field extends the region of electron crystal phase for extended system as was predicted by Lozovik&Yudson in 1975. Magnetic field influence on the crystal order in few-electron QD turns out to be more complicated. We have considered singlet-triplet transition controlled by interdot coupling. We investigate also possibility to control spin states of QD molecules by magnetic field.

S1X14 **Magnetic response of superconductor nanograins**

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For assemblies of superconductor nanograins, the magnetic response is analyzed as a function of temperature and magnetic field. In order to calculate the interaction energy of electron pairs for a huge number of the involved many-particle states, we develop an approximation, applicable over a wide range of the grain sizes and interaction strengths at arbitrary distributions of single-electron energy levels. Our study is focused upon ultra-small grains, where the nearest-neighbor spacing of single-electron energy levels can significantly exceed the bulk superconducting gap. For these grains, the overall profiles of the magnetic susceptibility as a function of magnetic field and temperature exhibit well-pronounced signatures of pairing correlations. The presence of these signatures does not depend on a particular choice of statistics, obeyed by single-electron energy levels in grains. This work has been supported by the GOA BOF UA 2000, IUAP, FWO-V projects Nos. G.0306.00, G.0274.01, G.0435.03, the WOG WO.025.99 (Belgium).

S1X15 **POLARON ENERGY SPECTRUM IN DISC SHAPED QUANTUM DOT**

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*1) Institute of Physics, Azerbaijan National Academy of Sciences*

It is known that the influence of polaron effect on carriers energy spectrum in semiconductors is enhanced both with decreasing of sizes and dimensionality of system from bulk to 2D, 1D and 0D. The normalized polaron energy shift for the ground state $\frac{\Delta E_0}{\alpha \hbar \omega_{L0}}$, where $\alpha$ is the coupling constant and $\hbar \omega_{LO}$ - the longitudional optical phonon energy, equals $-1$ and $\pi/2$ - for 3D and 2D systems, respectively. In 1D case $\frac{\Delta E_0}{\alpha \hbar \omega_{L0}}$ is proportional to $\ln R$ when the radius of the quantum wire $R \to 0$. The most significant polaron effects take place in quantum dots 0D. In this paper the polaron spectrum for disk-shaped QD was investigated using a modified perturbation theory. The oscillator model is used for the confining potentials in the forms $\frac{m\omega^2 \rho^2}{2}$ and $\frac{m\omega_z^2 z^2}{2}$, where $\omega_z >> \omega$. The using of the modified perturbation theory allows to determine the spectrum of the ground and excited states near the resonance points also, when the difference between energy levels is close to the optical phonon energy. The polaron shift diverges more sharply (as $R^{-1/2}$) than in the case of QWR when its radius tends to zero. The anticrossing of the polaron levels $E_1$ and $E_0 + \hbar\omega_0$ in the dependence of the QD radius was obtained near the resonance region. Far from resonance, the level $E_0 + \hbar\omega_0$ has no the particular physical meaning, however, the states corresponding to this level in the resonance region may be realized in experiments on light absorption. Apart from the allowed transition $E_0 \to E_1$, the transition $E_0 \to E_0 + \hbar\omega_0$ may also take place because the wave functions of these levels are mixed in the anticrossing region.

S1X16 **Contacting a Single Molecular Wire by STM Manipulation**

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*2) Nanoscience Group, CEMES-CNRS Toulouse, France*

The Lander molecule consists of a long polyaromatic main board maintained parallel above a surface by four TBP spacer groups. It represents a model system for investigating the electronic contact of a molecular wire to a nanoscale metallic electrode. Some recent manipulation experiments of single Lander molecules realized by STM at low temperature are presented, where the molecular wire part of a Lander is contacted to a monoatomic step and to a two atoms wide metallic nanostructure. The contact is characterized by the apparent height of the contact point in STM images and, in case of the Cu(111) substrate, by the perturbation observed in the electronic standing wave patterns. Moreover, the investigation of the standing wave pattern of a single Lander on a terrace show that specific information concerning the electronic interaction of the different internal groups of the molecule with the surface can be obtained.

S1X17 **Zeno effect and shot noise spectrum of superradiant entangled excitons**

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We consider two quantum dots embedded in a p-i-n junction. After a hole is injected into one of the quantum dot, the n-side electron can tunnel into the exciton level because of the Coulomb interaction. The noise spectrum can be calculated via the MacDonald formula. The double dot excitons are assumed to be in maximum entangled case, i.e. vanished sub-radiant decay rate. As will be shown, zero-frequency noise is enhanced by a factor of 2. This is analogous to the case of the single electron transistor near a Cooper pair resonance. Furthermore, the half-width of the spectrum is narrowed for strong measurements. One also finds both the occupation probabilities of singlet and triplet states grow with increasing the tunneling rate. This means quantum Zeno effect tends to destroy the entanglement.

S1X18 **AC conductance in the $p$-type Si/SiGe heterostructures with 2DHG**

G. O. Andrianov[1], I. L. Drichko[1], A. M. Diakonov[1], I. Yu. Smirnov[1], O. A. Mironov[2], M. Myronov[2], T. E. Whall[2], D. R. Leadley[2]
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The contactless acoustic method was applied for the first time in the strained $p$-type Si/SiGe heterostructures with sheet densities $p = 8 \times 10^{10}$ cm$^{-2}$ and $2\times10^{11}$ cm$^{-2}$. Measurements of attenuation and velocity of Surface Acoustic Waves (SAW) were carried out in the temperature range T=0.7 - 1.6 K, in magnetic fields H=0-7 T and in the frequency range 30-300 MHz to obtain high frequency conductivity and its dependence on H, T and SAW power. Degree of the carrier localization in this 2D system was traced using acoustics. The heating of a 2DHG in the Si/SiGe heterostructures by electric field of SAW was observed and analyzed. RFFI 04-02-16246.

### S1X19    **Photoluminescence in tetrahedral quantum dot quantum wells**

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High-resolution transmission electron microscopy has revealed that quantum dot quantum wells (QDQWs) are preferentially tetrahedral particles. Taking into account the tetrahedral shape of a QDQW when describing excitons, phonons and the exciton-phonon interaction, we obtain within a nonadiabatic approach [PRL **92**, 127402 (2004)] a quantitative interpretation of the photoluminescence (PL) spectrum of a single CdS/HgS/CdS QDQW. The exciton ground state in a tetrahedral QDQW is bright, in contrast to the dark ground state for a spherical QDQW. This work was supported by the GOA BOF UA 2000, IUAP, FWO-V projects G.0274.01, G.0435.03, the WOG WO.025.99 (Belgium), eiTT/COBRA, TU/e (The Netherlands), the MRDA-CRDF grant MP2-3044 (Moldova) and the EC GROWTH Programme, NANOMAT project G5RD-CT-2001-00545.

### S1X20    **Rashba effect in quantum networks**

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It has been recently shown that in a particular two-dimensional quantum network, the so called $\mathcal{T}_3$, quantum interference due to the Aharon-Bohm effect and to the topology of the network can induce strong localization [1,2]. For two-dimensional networks made up of quantum wires realized in semiconductor heterostructures, spin-orbit coupling due to the structural inversion asymmetry (Rashba effect[3]) may play an important role.
We study a quantum network extending in only one-dimension (chain of square loops connected at one vertex) made up of quantum wires with Rashba spin-orbit coupling. This system is a simplified version of a $\mathcal{T}_3$, and exhibits the same kind of localization when a magnetic field is applied. We show that the Rashba effect may give rise to a localization phenomenon similar to the one induced by magnetic flux. This localization effect can be attributed to the spin precession due to the Rashba effect. Furthermore, we study the effect of disorder on the transport properties of this networks. Finally, by means of simple consideration we are able to select the set of quantum networks where it is possible to achieve this phenomenon.
[1] J. Vidal, R. Mosseri and B. Douçot, Phys. Rev. Lett. **81**, 5888 (1998).
[2] C. Naud, G. Faini and D. Mailly, Phys. Rev. Lett. **86**, 5104 (2001)
[3] Yu A. Bychkov and E.I. Rashba, J. Phys. C: Solid State Phys. **17**, 6039 (1984).

### S1X21    **Spin-dependent transport through doped porphyrin molecular bridges**

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We consider several molecular bridges consisting of porphyrin monomers doped with various transition metals. These nanostructures are connected on their left and right to macroscopic gold contacts that are modeled by portions extracted from the Au(111) surface. Electronic transport characteristics of the bridges are calculated and compared. We make use of the surface Green's function matching approach in order to extend the left and right gold electrodes to infinity and obtain two semi-infinite contacts. The total Green's function of the whole system projected onto the bridge space is obtained. This readily results in the density of states and conductance characteristics of the nanodevice. The transport characteristics are obtained using ab initio modeling in a non-orthogonal basis. Possible practical applications are discussed.

## S1X22 **Novel Magnetic Properties of Atomically Arranged Perovskites**

B. Dabrowski[1]
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We have developed systematic strategy for making novel transition-metal perovskites AMO3 (A = Rare or Alkaline Earth's) with tunable magnetic and electronic properties. We show that for single-valent systems the magnetic superexchange interactions are dependent on average bond angle M-O-M. The structural disorder introduced by random substitutions on the A-site suppresses magnetic interactions through local deviations of bond angles. Similar disorder effects are enhanced for mixed-valent systems with double-exchange interactions. By stabilizing ordered structures; i.e., by suppressing local structural and charge disorder, an increase of magnetic transition temperatures of 100s K can be achieved. We demonstrate even more spectacular effects for the M-site ordered perovskites with transitions from spin-glass to 600 K ferromagnets. To obtain these compounds we have developed special synthesis techniques and developed design rules based on tolerance factor that depends on composition, temperature, and oxygen content.

## S1X23 **Effect of B-site substitution in the perovskite phase CaMnO$_3$**

R. P. Borges[1], P. G. Gião[2], M. D. Carvalho[2], M. M. Cruz[1], M. Godinho[1]
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Manganese perovskite structures AMnO$_3$ have regained new interest due to their magnetoresistive properties. The presence of a mixed valence state for manganese ($Mn^{3+}/Mn^{4+}$) and the existence of a ferromagnetic ordered state are ingredients now considered essential to have important magnetoresistive behaviour. Most of the work carried out in the search for optimal compositions has been based on the substitution of the A-cation. Recently the doping in octahedral structural site (Mn site) by magnetic ions has been tried in order to tune the effect leading to some promising results. In this work we studied the influence of manganese substitution for vanadium in the perovskite phase CaMnO$_3$. The higher oxidation state of V ions reduces some $Mn^{4+}$, with consequent influence on the properties of the samples. A significant ferromagnetic phase is observed for all doped samples but T$_C$ decreases with increasing V content.

## S1X24 **MANGANITES WITH Eu AND Ce: TRANSPORT AND MAGNETIC PROPERTIES**

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First time Eu$_{1-x}$Sr$_x$MnO$_3$ single crystals have been grown. Resistivity, magnetic susceptibility and magnetization of ceramic and single crystal samples of Eu$_{1-x}$MnO$_3$, Eu$_{1-x}$Sr$_x$MnO$_3$, La$_{1-x}$Ce$_x$MnO$_3$, and La$_{0.7}$Ce$_{0.15}$Ca$_{0.15}$MnO$_3$ were studied. In the Eu doped manganites low temperature antiferromagnetic ordering was observed. Magnetic susceptibility peak temperature position and form depend on $x$, external magnetic field and on the sample nature - ceramic or single crystal. The manganites Eu$_{1-x}$Sr$_x$MnO$_3$ resistivity decreases with $x$ increasing. For $x$=0.3 the insulator-metal transition in magnetic field was observed. A low temperature anomaly of the magnetic susceptibility and the magnetization were observed for the La$_{1-x}$Ce$_x$MnO$_3$ manganites. An increase of Ce concentration in the perovskite phase leads to a corresponding decreasing of the antiferromagnetic coupling between Mn spins and the samples resistivity. The last one can be considered as indirect evidence of $Ce^{4+}$ ions presence in the perovskite phase.

S1X25 **NMR studies of PrCu$_2$**

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We present the first results of NMR measurements of PrCu$_2$, an intermetallic compound which exhibits a number of low temperature phase transitions.
We observe that between 20 and 300 K, the temperature evolution of the Knight shifts of the $^{63}$Cu- and $^{65}$Cu NMR lines follow a Curie-Weiss type behavior, as expected for an NMR response dominated by the 4f-electron magnetic moments of the Pr$^{3+}$ ions. At temperatures above 100 K, the $^{63,65}$Cu-NMR spectra exhibit the characteristic powder pattern for a nuclear spin $I = \frac{3}{2}$, as expected for Cu nuclei in a noncubic environment. Significant changes in the NMR spectra are observed between 20 and 100 K. They may be interpreted as evidence for either (i) a complicated antiferromagnetic order, and/or (ii) substantial changes in the internal distribution of electric charges.

S1X26 **Magnetic and electronic structure of La$_{0.7}$Sr$_{0.3}$MnO$_3$/Sr$_2$FeMoO$_6$ interface**

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We present theoretical calculations of the electronic and magnetic structure of the interface between La$_{0.7}$Sr$_{0.3}$MnO$_3$ and Sr$_2$FeMoO$_6$. The calculation where performed for an ideal interface using the GGA approximation. Bulk La$_{0.7}$Sr$_{0.3}$MnO$_3$ and Sr$_2$FeMoO$_6$ are considered to be minority spin and majority spin half metals respectively and the calculation show that the interface essentially have bulk electronic structure two atomic layers from the interface. The calculations show that the magnetization directions of the interface are parallel which imply anti paralell alignment of the spin directions of the electrons at the Femi level close to the interface. We speculate that the interface will show negative CMR in contrast to the bulk of La$_{0.7}$Sr$_{0.3}$MnO$_3$ and Sr$_2$FeMoO$_6$

S1X27 **Magnetic and mechanical properties of Fe$_3$Pt and FePt$_3$**

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An ab initio study of magnetic and mechanical properties of Fe$_3$Pt and FePt$_3$ along the tetragonal deformation path is presented. Total energies, magnetic moments and bulk moduli are calculated using the state-of-the-art full potential linearised augmented plane waves (FLAPW) method. All calculations are performed within the general gradient approximation (GGA). Total energies are displayed in contour plots as functions of tetragonal distortion and volume; borderlines between the ferromagnetic, antiferromagnetic and nonmagnetic states are shown. The calculated results are compared with available experimental data.

S1X28 **Electrical transport properties of UPtAl under ultra high pressure**

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UPtAl is a ferromagnet with Curie temperature $T_C$ =42.5K and spontaneous magnetic moment $M_s$ =1.4 $\mu_B$ /f.u. The temperature dependence of $R(T)$ in the ferromagnetic state can be elucidated by spin-wave spectrum with an energy gap $\Delta \sim$ 60K. In the present work, we have explored the development of magnetic and electronic properties of UPtAl under high pressure up to 22 GPa by measurements of electrical resistivity, which exhibits a the typical anomaly at 42.5 K, which we take as a label of $T_C$. The $T_C$ value initially increases and peaks at 6 GPa. Finally, we have observed a considerable change of electronic structure for p $\leq$ 17 GPa expressed by: i)$R(T)$ looses the characteristic feature at $T_C$ and it shows only a broad shoulder around 25 K, ii)residual resistivity shows maximum, iii)$T^2$ coefficient of $R(T)$ seems diverges and iv)$\Delta$ is almost suppressed.

S1X29 **Antiferromagnetic domain walls in lightly doped layered cuprates**

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Recent ESR data [1] shows rotation of the antiferromagnetic (AF) easy axis in lightly doped layered cuprates upon lowering the temperature. I account for the ESR data and show [2] that it has significant implications on spin and charge ordering according to the following scenario: In the high temperature phase AF domain walls coincide with (110) twin boundaries of an orthorhombic phase. A magnetic field leads to annihilation of neighboring domain walls resulting in antiphase boundaries. The latter are spin carriers, form ferromagnetic lines and may become charged in the doped system. However, hole ordering at low temperatures favors the (100) orientation, inducing a $\pi/4$ rotation in the AF easy axis. The latter phase has twin boundaries and AF domain walls in (100) planes.

1. A. Jánossy, T. Fehér and A. Erb, Phys. Rev. Lett. **91**, 177001 (2003).
2. B. Horovitz, Phys. Rev. B **69**, 140501(R) (2004).

S1X30 **Development of magnetism in U(Ni,Pd)$_2$Si$_2$ under pressure**

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UPd$_2$Si$_2$ shows at low temperatures the magnetic ordering of AF$-$I type, which consists of basal-plane ferromagnetic layers of U moments aligned along the $c$-axis, whereas UNi$_2$Si$_2$ condensates in the uncompensated antiferromagnetic (UAF) structure with the $++-$ coupling. We report on results of our magnetization, resistivity and neutron-scattering studies of evolution of magnetic ground state of U(Ni$_{1-x}$Pd$_x$)$_2$Si$_2$ compounds at ambient and high hydrostatic pressure. The volume fraction of the AF$-$I phase increases with increasing $x$. On the other hand, the hydrostatic pressure and magnetic field promote the UAF phase.

S1X31 **Hyperfine fields distribution in bcc binary Fe-based disordered alloys**

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BCC binary $Fe_{1-x}M_x$ (M = V, Nb, Mo, Ta) disordered alloys have attracted interest due to a number of peculiar magnetic properties. In $Fe_{1-x}M_x$ for small concentrations $x$ the M atom possesses an induced magnetic moment, which is of about $1\mu_B$ for V and $0.5\mu_B$ for Nb, Mo and Ta. With $x$ increasing the atomic magnetic moments decrease and for $x > 0.5$ the alloys become nonmagnetic. The atomic magnetic moment calculations give us pertinent information about the type and the value of magnetic coupling between atoms in an alloy. Additional and important information may be deduced from hyperfine field calculations.
In this contribution, we report on a theoretical study of hyperfine fields in $Fe_{1-x}M_x$ alloys. According the decomposition of the electronic system one can separate the contribution to the hyperfine field of the core and the band valence electrons. As it is known, there is not a strict relationship between magnetic moment and hyperfine field. Nevertheless, calculations of the concentration dependences of the different $l$-contributions into $\mu$ and $B^{core(val)}$ allowed us to poin out fair correlations between $B_{s(p)}^{core}$ and $\mu_{spin,d}$ as well as between $B^{val}$ and $\mu_{spin,s}$ for all considered compounds.

S1X32 **Spin Wave Spectra in Fe/Cr(100) Ultra-Thin Films**

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In this work we have calculated the ferromagnetic resonance curves of Fe/Cr (100) thin films, which follow the Fibonacci sequence. Our approach is based on the equations of motion for the small-signal magnetization deviation from the equilibrium directions. In addition to the bilinear and biquadratic exchange, our theory takes full account of surface, in plane uniaxial, and cubic anisotropy interactions. We consider also the presence of an external magnetic field applied in the plane of the films and parallel to the easy axes. Our theoretical predictions are adequate to extract reliable values for the magnetic parameters involved, since the frequencies of the magnetic excitations depend directly upon the magnetization configuration of each ferromagnetic. Our calculations are adequate to low wave number spin waves, and the analytical expressions derived here can be observed in either BLS experiments or FMR techniques.

S1X33 **Structural and magnetic phase diagram of SmS under pressure**

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Recently SmS has seen a resurgence of interest as it provides an opportunity to study a magnetic Quantum Critical Point, close to a valence instability. Magnetic order has already been found to occur for pressures above 2GPa. This work clarifies several points in the low temperature/high pressure phase diagram. We present X-ray structural and absorption edge measurements at low temperature where the pressure is changed in-situ. This allows the first determination of the Sm valence within the magnetically ordered phase, and shows that magnetic order sets in well before Sm becomes trivalent. We also present high pressure calorimetry experiments which prove that the magnetic order is long range, and give a better determination of the magnetic phase diagram.

S1X34 **Magnetic properties of the ternary Laves-phase $(Zr,Mn)Co_{2+\delta}$ compounds.**

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The binary Laves-phase compounds $ZrCo_2$ and $ZrMn_2$ are Pauly paramagnetic. The spontaneous magnetization was observed in nonstoichiometric $ZrCo_{2+x}$ compounds with x$\geq$0.8 and the $T_c$ of them reached up 160 K. Curie temperature (Tc) of the ternary $Zr_{1-x}Mn_xCo_{2+\delta}$ compounds is about 600 K and the magnetization is 100 emu/g at room temperature. For that using the X-ray and neutron powder diffraction we studied the crystal and magnetic structure of $Zr_{1-x}Mn_xCo_2$ and $Zr_{1-x}Mn_xCo_{2.45}$ system compounds. We found that $Zr_{0.8}Mn_{0.2}Co_2$ compound crystallized in the $MgCu_2$ type cubic structure, (Fd3m space group). These $Zr_{0.64}Mn_{0.36}Co_2$ and $Zr_{0.64}Mn_{0.36}Co_{2.45}$compounds crystallized in the $AuBe_5$ type cubic structure, (F-43m space group). All the compounds are ferromagnetic. An appearance of the ferromagnetism in $Zr_{1-x}Mn_xCo_{2+\delta}$ alloys can be considered, within the scope of a model of the itinerant electrons.

S1X35 **Magnetic structure of itinerant antiferromagnet $UGa_3$**

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$UGa_3$ orders in a rather simple magnetic structure with U moments aligned antiferromagnetically in adjacent (111) ferromagnetic planes. Recently it was found (Nakamura et.al., J. Phys. Chem. Sol. **63** (2002), 1193), that magnetic moments are parallel to [110] direction. We performed *ab initio* calculations in the framework of Density Functional Theory of this system. We treated uranium f-electrons as ordinary band electrons in local density approximation. In order to better describe these correlated states we employed LSDA+U treatment. Our results reproduce magnitude and direction of observed magnetic moments.

S1X36 **On the influence of the density of states form on ferromagnetism in doubly degenerate Hubbard model**

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In this work for the case of strong intra-atomic Coulomb and Hund couplings with use of perturbation theory the effective Hamiltonian of doubly orbitally degenerate band is obtained. With use of the projection procedure in the Green function tecnique the quasiparticle energy spectrum is obtained. The peculiarity of the obtained spectrum is the spin-dependent shift of band center with the magnitude dependent on unperturbed density of states. The performed calculation of the ground state energy has allowed us to calculate critical concentrations at which magnetization occurs and saturates for different forms of density of states as well as to obtain the concentration dependencies of system magnetization. In the case of orbitally degenerate band ferromagnetism can be realized by translational mechanism.

S1X37 **Anomalous magnetic phase in $Ho_{1-x}Y_xB_2C_2$**

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The tetragonal $HoB_2C_2$ shows antiferroquadrupolar order (AFQ) transition at $T_Q = 4.5$ K. This transition occurs below the antiferromagnetic (AFM) transition temperature $T_N = 5.9$ K. In order to investigate the origin of this unusual AFM phase appearance, we try changing the strength of interactions in $HoB_2C_2$ by substituting $Y^{3+}$ for $Ho^{3+}$. Elastic properties of $Ho_{1-x}Y_xB_2C_2$ have been studied by means of ultrasonic measurements. The anomalous softening of elastic constants was reported in the AFM phase for $HoB_2C_2$. Although the $x = 0.40$ sample shows no evidence of $T_Q$ at least down to 0.5 K, the similar anomalous softening is observed below $T_N$.

S1X38 **Original magnetic behavior of the compounds $Ce_2Fe_{17-x}Mn_x$ and their hydrides**

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Large variety of magnetic ground states was observed in $Ce_2Fe_{17-x}Mn_x$ ($x \leq 2$) compounds: the collinear ferromagnetic one at $x < 0.5$ ($T_C \leq 94$ K), the antiferromagnetic one at $0.5 \leq x \leq 1$ and noncollinear structure with ferromagnetic component at $x > 1$. The Neel temperature decreases from 204 to 174 K with Mn content. In this contribution, we will review the original properties of these materials and our recent results of the effects of external pressure and insertion of Hydrogen. We found that transition to ferromagnetic state can be induced both by expansion (introduction of H) and by compression (under pressure) of crystal lattice that can indicate complex changes of electronic structure under these effects.

S1X39 **Ab initio study of nickel magnetism along the Bain deformation path**

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We present a study of magnetic behavior of nickel along the tetragonal (Bain) deformation path at various atomic volumes. The total energies are calculated by full-potential linearized augmented plane waves (FLAPW) method incorporated in the WIEN2k code. Magnetic ordering is taken into account by means of a spin-polarized calculation. Two approximations for the exchange-correlation term are employed: the local (spin) density approximation and the generalized gradient approximation. Calculated total energies are displayed in contour plots as functions of tetragonal distortion c/a and volume. Borderlines between various magnetic phases are shown. Detailed comparison of the LDA and GGA results is performed.

S1X40 **The Phase Diagram of Magnetic States in the Ferromagnetic Nanoparticle with Single-Ion Anisotropy.**

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Superparamagnetic state is observed in inhomogeneous condensed matter, which includes isolated ferro- or ferrimagnetic nanoparticles with $N=10^3 - 10^5$ magnetic atoms. The phase diagram of magnetic states was studied for the isolated nanoparticle with ferromagnetic intraparticle exchange interaction and single-ion uniaxial anisotropy of second order and quantum atomic spins S=1. It was shown, that for the case of easy-axe anisotropy (parameter of anisotropy D>0) at the lowering temperature the transition is observed from paramagnetic state to the superparamagnetic state of Ising-type, and for the case of easy-plane anisotropy (D<0) to the superparamagnetic state of XY-type. The details of transition temperatures shift to these states are studied for the different orientations of external magnetic field to the anisotropic axe.

## S1X41 **Random competing interactions in perovskites**

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Magnetic measurements, such as magnetic hysteresis, have been performed for perovskites randomly doped with Ce atoms. Loops show partially reproducible hysteresis cycles. At very weak fields (under 50 Oe) a step-like behavior is found with jumps in the magnetization at certain values of the external magnetic field. This is probably due to random competing interactions whose origin is discussed. An Ising Hamiltonian including a mixture of ferromagnetic and antiferromagnetic interactions on a simple cubic lattice is tried on showing that some of the features of the experimental cycles can be reproducerd by means of a Monte Carlo simulation. Temperature dependence is also mimicked and discussed. Further developments of this phenomenon are brought out.

## S1X42 **Preparation and magnetic properties of the layered compound CeRuPO**

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Two-dimensional systems have attracted considerable attention in the past years. Compounds of the type LnRuPO (Ln=Rare-Earth) have a rather unusual crystal structure with alternating layers of RuP4 and OLn4 tetrahedra making them intermediate systems between inter-metallics and oxides. Though first synthesised about a decade ago, little is known about their physical properties. We were interested in CeRuPO, since its cell volume shows an anomalous contraction compared to other LnRuPO compounds, suggesting an unstable Ce-valance state. Here we present the preparation and the first report of the physical and magnetic properties of this compound. The sample shows a Curie-Weiss behaviour at high temperatures with $\theta_P$=15K and $\mu_{eff}$=2.3$\mu_B$ and undergoes a ferromagnetic transition at 20K. These results along with other physical properties such as resistivity and specific heat will be discussed in the presentation.

## S1X43 **On magnetic helicoidal structures**

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Theoretical research of magnetic helicoidal structures, including multiple spin-density wave states, is carried out by means of the original approach. The proposed method and results of investigation are compared with those ones obtained by known alternative methods. Relevant spectroscopic data are analysed briefly and compared with typical commensurate magnetic phases. This research is supported by NATO (PST.CLG979685) and Ministry of Education and Science of Ukraine (M352/2003).

S1X44 **Calculated de Haas-van Alphen quantities of Ce$M$In$_5$ ($M$ =Co, Rh, and Ir)**

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We report a critical analysis of the electronic structures and de Haas-van Alphen (dHvA) quantities of the heavy-fermion superconductors CeCoIn$_5$, CeRhIn$_5$, and CeIrIn$_5$. The electronic structures are investigated *ab initio* on the basis of full-potential band-structure calculations, adopting both the scalar- and fully relativistic formulations within the framework of the local spin-density approximation (LSDA). We compare our calculated dHvA quantities with other recent relativistic calculations and discuss the differences between them.

S1X45 **SrZnVO(PO$_4$)$_2$: strong frustration in a ferromagnetic square lattice**

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Frustrated square lattices (FSL) are of interest because they can be driven to a quantum critical state by tuning the frustration ratio $\alpha = J_2/J_1$. SrZnVO(PO$_4$)$_2$ is structurally close to Pb$_2$VO(PO$_4$)$_2$, the first reported ferromagnetic FSL compound. We performed the first physical study on SrZnVO(PO$_4$)$_2$ by means of susceptibility $\chi$(T) and specific heat C$_p$(T) measurements. $\chi$(T) shows a clear maximum at T$_{Max} \simeq 6.2$ K and a kink at T$\simeq$2.7K where a magnetic phase transition towards a long range ordered state takes place. Fitting $\chi$(T) with a high-temp. expansion series lead to exchange param. J$_1 \simeq -8.3K$ and J$_2 \simeq 8.9K$ ($\alpha \simeq -1.1$), i.e. a nearest-neighbor ferromagnetic interaction and a slightly larger antiferromagnetic exchange along the diagonal between next-nearest-neighbors as in Pb$_2$VO(PO$_4$)$_2$ ($\alpha \simeq -1.8$). This value of $\alpha$ places SrZnVO(PO$_4$)$_2$ close to the critical point $\alpha = -0.5$ where fluctuation effects should be important.

S1X46 **US : Exchange Interactions and Curie Temperature**

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In recent years, there has been a growth in interest in the calculation of ground state (T=0) exchange parameters and an analysis of the Curie temperature. A common technique involves the analysis of spin spirals (magnons) in order to deduce the exchange parameters, the implementation of which is easiest without spin orbit coupling. This approach has worked well for many compounds, however for US the neglect of s.o. coupling is a severe limitation. Here, results are presented for the exchange parameters of US, including spin orbit coupling, deduced within a supercell approach. The accuracy of the supercell is analysed via comparison (in the limit of no spin orbit coupling) with the "spin spiral" approach.

**S1X47** **The role of exchange anisotropy and uniaxial single-ion anisotropy in a magnetic behaviour of spin-1 dimer**

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Magnetic properties of a spin-1 dimer are exactly determined in order to clarify the role of exchange and single-ion anisotropies, which may basically influence the magnetic behaviour. Interestingly, such a simple system as the spin-1 dimer may exhibit a very rich magnetic behaviour. In fact, a variety of spin arrangements were found for both ferro- and antiferromagnetic spin-1 dimers depending on a ratio between exchange and single-ion anisotropies, magnetic field and exchange constant. Among other matters, an exact evidence for a magnetization process with a single-plateau magnetization curve is found, in addition to a standard double-plateau magnetization curve. A possible experimental realization of the model under investigation represents a special class of real molecular-based $Ni_2$-dimer compounds, a connection between theory and experiment will be presented.

**S1X48** **MAGNETIC STRUCTURES IN CUBIC $RCu_5$ (R=Tb, Dy, Ho) COMPOUNDS**

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The magnetic and structural properties of melt spun $RCu_5$(R=Tb, Dy, Ho) with the cubic $AuBe_5$ type structure have been investigated with the neutron diffraction and magnetic measurements. Samples consisting of small polycrystalline plates of $RCu_5$ have been measured in a magnetic field up to 5 T and for temperature range 1.7-50 K. In magnetisation measurements it has been found that $TbCu_5$ and $DyCu_5$ behave antiferromagnetically below a temperature of 15 K and 7 K, respectively. In zero magnetic field the magnetisation of $HoCu_5$ shows also a sharp maximum at 3 K characteristic for antiferromagnetic ordering, but below 3 K the dependence of the magnetisation on an applied magnetic field is typical for ferromagnetic materials. For R=Tb an antiferromagnetic of G-type structure in the fcc lattice was determined by neutron diffraction experiments at 4.2 K [1]. Our measurements confirm these results but we performed the measurements at different temperatures and in an applied magnetic field. The $HoCu_5$ sample did not show long range magnetic order in zero field. At 2 K and at magnetic fields greater than 0.5 T ferromagnetic peaks were found.
[1] T. Kaneko et al., J. Magn. Magn. Mater. 54-57 (1986) 469

**S1X49** **Influence of interface alloying on the magnetic properties of Co/Pd multilayers**

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An important issue concerning Co/Pd multilayers is the origin of their perpendicular anisotropy: broken symmetry at the Co/Pd interface or magnetoelastic effects in an interfacial CoPd alloy? We studied multilayers with the structure: $\{(Co-3 \ \mathring{A}$ co-deposited with Pd-y $\mathring{A}) /$ Pd-(20-y) $\mathring{A}\}_{15}$, with y=0,1,3,5,10,15,20. Magnetic properties are almost unaffected by the alloying up to y=5 $\mathring{A}$. The interface of the usual Co/Pd multilayer could be thus modeled by a mix of 3 $\mathring{A}$ of Co with 5 $\mathring{A}$ of Pd. The magnetoelastic effet using such a picture would yield to a perpendicular anisotropy between 2.3 and $3.5 \times 10^6$ erg/cm$^3$, in good agreement with the one measured in our samples.

S1X50 **Ideal tensile strength of ground-state and higher-energy structures in Fe$_3$Al**

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Magnetic behavior of Fe$_3$Al in the ground-state structure D0$_3$ and in a hypothetic structure L1$_2$ was studied along the trigonal deformation path from first principles, using the FLAPW method (the WIEN2k code). For the exchange-correlation energy, both the local density approximation (LDA) and the generalized gradient approximation (GGA) was employed. The hypothetic structure L1$_2$ was found to be non-magnetic in contrast to the feromagnetic D0$_3$ structure. Moreover, the ideal tensile strength of both structures for tensile loading along the [111] direction was determined. Total energies were displayed in contour plots as functions of trigonal distortion and volume; a path corresponding to the uniaxial tensile test is also exhibited.

S1X51 **YFe$_4$Al$_8$: spin spiral or modulated moments?**

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Ternary compounds MFe$_4$Al$_8$, (M = Rare Earth, Actinides), with ThMn$_{12}$ structure type show a large variety of magnetic properties. For YFe$_4$Al$_8$ two neutron diffraction studies proposed differing magnetic structures: a spin spiral and a moment modulated structure. In order to clarify the magnetic structure of YFe$_4$Al$_8$ Density Functional Theory calculations were performed, within the Local Density Approximation, using the Augmented Spherical Waves method modified to account for spin spiral structures. Several spin spiral structures were analysed, including ferro and antiferromagnetic structures. The results show that the AFM structure has lower energy than any of the spin spirals considered in the calculations.The calculations were extend to modulated structures, using a supercell. The possible magnetic structures are discussed making direct comparison between modulated and spin spiral structures.

S1X52 **High quality ultrathin Fe films on Ge(001): towards the control of the electronic and magnetic properties**

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The Fe/Ge(001) interface is a very attractive system for growing well ordered epitaxial FM/SC etherostructures. Spin dependent interface resistance plays a crucial role in spin injection in semiconductors (SC) from ferromagnets (FM), and it is strongly related to the real interfacial properties. We have then investigated ultrathin Fe layers, grown at room temperature, that display no sizable intermixing and magnetic dead layer: the onset of ferromagnetic order is definitively found at Fe thickness of 3 ML. All the films display an uniaxial anisotropy: its direction, together with the electronic and magnetic properties of Fe films, can be controlled by tuning the geometrical parameters involved in the sample preparation and by employing virtual Si$_x$Ge$_y$ substrates with different lattice parameters.

S1X53 **Colossal Magnetoresistance and Percolation Effects in $Eu_xCa_{1-x}B_6$**

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Upon substituting Ca for Eu in the local-moment ferromagnet $EuB_6$, the Curie temperature $T_C$ decreases substantially with increasing dilution of the magnetic ions, resulting in a spin-glass ground state for $x \leq 0.3$. The Ca substitution leads to significant changes of the electronic properties at low temperatures across the $Eu_xCa_{1-x}B_6$ series. Electron microscopy data for $x \approx 0.27$ indicate among a high structural perfection of our samples also an electronic phase separation into Eu- and Ca-rich clusters of 5 to 10 nm diameter. This clustering leads to percolation-type phenomena in the electrical transport properties. Close to but below the related critical concentration of $x_p \approx 0.3$, we observe colossal negative magnetoresistance effects at low temperatures, similar in magnitude as those reported for manganese oxides.

S1X54 **Magnetism of $Y_2Fe_{17}$ under high pressure up to 10 GPa**

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Considerable non-linear decrease of magnetization and Curie temperature at pressures above 0.6 GPa, large anisotropic magnetovolume anomalies and peculiar behavior of a.c. susceptibility are indications of volume instability of ferromagnetic structure and/or magnetic moments of Fe. To clarify an origin of these effects we performed neutron diffraction experiments on $Y_2Fe_{17}$ up to 10.2 GPa in the temperature range 4-280 K. Incommensurate helical antiferromagnetic structure has been discovered at pressure above 1 GPa. It is remarkably stable under high pressure and even at 10 GPa the magnetic order exists up to 200 K. The fundamentals of the pressure phenomena can be connected with different volume dependence of Fe-moments in four inequivalent crystallographic positions and/or with anisotropic exchange interactions.

S1X55 **Optical studies of alpha-MnS under high pressure**

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The discovery of the colossal magnetoresistance in (FeS)-(MnS) solid solutions revived interest of MnS, which is the basic component of these substances. An alpha-MnS possesses an NaCl type cubic lattice and an antiferro-paramagnetic phase transition occurs at 150 K. In high pressure region, some X-ray studies have been performed previously. However their results are not consistent and the transition pressure is not clear until now. We performed the absorption and reflection measurements in alpha-MnS under high pressure at room temperature. With increasing pressure, absorption edge reaches to 0 eV around 26 GPa and then the reflectivity increases drastically. Therefore it is concluded that the phase transition in alpha-MnS occurs at 26 GPa is the semiconductor-metal transition.

S1X56 **Magnetic ordering of $Ce_2Fe_{17-x}Mn_x$ with $x \geq 1$ under pressure**

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Magnetization and neutron diffraction measurements under pressure were performed on $Ce_2Fe_{16}Mn$ and $Ce_2Fe_{15.3}Mn_{1.7}$ compounds in order to clarify the origin and magnetic structure of the re-entrant ferromagnetic phase in $Ce_2Fe_{17-x}Mn_x$ with $x \geq 1.3$ and its possible correlation with the pressure induced magnetic phase in $Ce_2Fe_{16}Mn$. The obtained results indicate relatively high stability of the pressure induced magnetic phase to the volume changes. Neutron diffraction experiments confirmed the identity of the pressure induced phase in $Ce_2Fe_{16}Mn$ and the re-entrant ferromagnetic phase in $Ce_2Fe_{15.3}Mn_{1.7}$ at ambient pressure.

S1X57 **Thermomagnetic effects in direct-gap HgCdSe semiconductors under hydrostatic pressure**

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In the present work both the thermoelectric and galvano and thermomagnetic (longitudinal and transverse Nernst-Ettingshausen) effects were investigated in single crystals of gapless semiconductors $Hg_{1-x}Cd_xSe$ (x=0, 0.03, 0.07) at hydrostatic pressure conditions up to 2 GPa. From the effects mentioned the pressure dependencies of concentration and mobility of charge carriers have been estimated. The thermomagnetic effects are known to be preferable in compare with galvanomagnetic ones for analysis of electron structure and charge carriers scattering mechanisms as well as their variation at high pressure. The work was supported by the RFBR, Gr. No. 04-02-16178, and INTAS (Ref. Nr. 03-55-629).

S1X58 **Thermoelectric properties at ultrahigh pressure of doped p-PbTe-based single crystals**

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In the present work the thermoelectric and electric properties have been investigated of semiconductor microsamples based on p-PbTe compounds (Pb1-xGaxTe, Pb1-xSnxTe, Pb1-xSixTe, Pb1-xMnxTe, PbTe1-y, Pb1-yTe, (Pb1-xSnx)1-yTe) at ultrahigh pressure up to 20 GPa. For some compositions the sign inversion of thermopower (traditional for p-type lead chalcogenides PbSe, PbS) have been observed before NaCl-GeS phase transition; also it was noted a shift of NaCl-GeS structural phase transition pressure on content of impurity. Whereas, for other compositions some anomalies (absence of inversion sign of thermopower, stabilization of thermopower value in a wide range of pressure, strong irreversible changes of thermopower due to pressure treatment, etc.) have been observed. The work was supported by the RFBR Gr. No. 04-02-16178, and INTAS (Ref. Nr. 03-55-629).

**S1X59** **Pressure induced transformations in metallic and semiconducting carbon nanotubes**

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Due to their unique one dimensional structure carbon nanotubes are expected to stand up, through pressure application, strong geometrical changes. This has motivated an important number of experimental and theoretical investigations. Motivated by these considerations, we take profit of the resonant selectivity of Raman spectroscopy to separately study the high pressure evolution of metallic and semiconducting carbon nanotubes, by working at two different excitation wavelengths for pressure up to 40 GPa. Both types of nanotubes show a phase transition at 10 GPa suggesting the independence of the transition pressure with tube chirality. Two different high pressure phases are observed showing either a normal carbon-like compression or a pure bending response. We show that the disappearance of the radial modes at pressures below 10 GPa is related to the resonant character and not to a structural transition.

**S1X60** **FM-AFM crossover in $TbPt_{1-x}Cu_x$ studied under pressure**

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The series $TbPt_{1-x}Cu_x$ presents a change of the magnetic behaviour with increasing Cu content and a negligible volume change: the compounds with Cu concentrations x<0.3 present a ferromagnetic character; on the contrary, for x>0.3, we found a global antiferromagnetic behaviour corresponding to complex magnetic structures. For the intermediate compound, $TbPt_{0.7}Cu_{0.3}$, an evolution from an AFM to FM, stable until very low temperatures, is observed. We present pressure effects on the magnetic behaviour of the $TbPt_{1-x}Cu_x$ series studied by susceptibility measurements up to 10 kbar. These results are discussed in relation with neutron diffraction under pressure.

**S1X61** **Influence of PT pre-treatment on thermoelectric properties of Czochralski grown silicon in pressure range 0-20 GPa**

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Characterization of silicon is an actual problem both for its micromachining and for microelectronics [1]. Single crystalline Si rods are usually grown by Czochralski (Cz) technique. Czochralski-grown silicon (Cz-Si) contains interstitial oxygen which redistributes at annealing both into electrically active oxygen containing clusters and into electrically passive precipitates associated with structural defects. In the present paper the technique of thermoelectric measurements at ultrahigh pressure has been applied for characterisation of Cz-Si pre-treated for 10 h at 450C, 600C and 650 C under various hydrostatic pressures (0.01, 0.1, 0.6 and 1.4 GPa) of argon gas. Thermopower and electrical resistance of these samples have been measured at ultrahigh pressure P up to 20 GPa. The semiconductormetal structural phase transitions and values of thermopower of high pressure phases have been established.The authors are grateful to the Russian Foundation for Basic Research (RFBR) for financial support of the work (Gr. No. 04-02-16178).[1]V.V. Shchennikov, S.V. Popova, A. Misiuk. Technical Physics Letters, 2003, 29, 598-601.

S1X62    **<u>Suppression of the martensitic transformation in TbCu and GdCu induced by pressure</u>**

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The equiatomic RCu (R=Gd, Tb) compounds undergo a martensitic transformation evolving from a cubic CsCl-type of structure at room temperature to a mixture of cubic and orthorhombic phases at lower temperatures. We report the effects of pressure on this martensitic transformation studied by means of thermal expansion and electrical resistivity. We have found that this transformation is very sensitive to pressure, especially in TbCu, where 0.3 GPa are enough to suppress it. In addition X-ray diffraction under pressure experiments showed that at room temperature, the cubic phase is stable up to 13 GPa and 17 GPa in GdCu and TbCu respectively, evolving to a lower symmetry phase at higher pressures.

S1X63    **<u>Modeling of intermolecular interaction potentials in dense gaseous medium based on ab initio calculations</u>**

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Analytic intermolecular or atom-atom interaction potentials of small molecules allow to calculate the parameters of state of dense gaseous medium (planetary atmospheres, detonation products, etc). In the first case the molecules are considered as a point interaction centers, in the second case the real molecule geometry is preserved. This paper presents a way to construct the EOS for dense gas on an example of molecular nitrogen, based on quantum mechanical interaction energy calculations of molecular configurations consisting of two or several molecules with various distance between centers of gravity and various mutual orientations. The parameters of pair atom-atom EXP6-potential, reproducing ab initio calculations, were defined by the least square method on a large number of configurations, as well as the parameters of effective pair potential which includes many-particle interactions.

S1X64 **Pressure-induced photoluminescence in MnF$_2$ at Room Temperature.**

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We have recently shown that photoluminescence (PL) and non-radiative processes yielding PL quenching in Mn$^{2+}$-doped fluorite crystals (Ca$_{1-x}$Sr$_x$F$_2$) mainly depend on the host site volume. The smaller the volume, the higher the PL efficiency [1]. Following this idea, we were able to induce PL at room temperature (RT) in the non-PL Mn$^{2+}$-doped SrF$_2$ and BaF$_2$ using high-pressure techniques [2].

On the other hand, the PL mechanism is quite different in concentrated materials such as MnF$_2$ (rutile-type structure). PL takes place in Mn$^{2+}$-perturbed traps after excitation migration. In this system, however, PL occurs only at low temperatures given that is quenched for T > 100 K thus not being luminescent at RT [3].

In this work we demonstrate that non-PL MnF$_2$ can be transformed to PL MnF$_2$ by pressure. We observe a strong correlation between the appearance of RT PL and the pressure induced structural changes (the phase transition sequence is rutile → distorted fluorite → cotunnite) [4]. We observe two PL centres for P > 14 GPa whose emission bands peak at 2.34 eV and 1.87 eV and are likely associated with Mn$^{2+}$ intrinsic PL and Mn$^{2+}$ perturbed traps, respectively. Thus, pressure reveals as an efficient tool to reduce the excitation migration since excitation can be more efficiently retained in Mn$^{2+}$ traps or even non-perturbed Mn$^{2+}$ thus increasing the PL efficiency of the material at a given temperature. Interestingly, the present findings open new ways of achieving PL based on concentrated materials, particularly, in those cases where phase transformations show large hysteresis. The results are compared with the spectroscopic studies carried out in MnF$_2$ nanocrystals obtained by milling [5] as a function of temperature and pressure.

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S1X65 **Magnetic moment of Iron under high pressure**

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Anomalous magnetovolume phenomena in Fe-rich alloys, like Invar and anti-Invar effects, martensitic transitions and shape memory effects, have been understood and described from the first principles just recently. The origin of the anomalies was related to an electron transfer between antibonding and non-bonding states close to the Fermi level and to a relevant shrinkage of the crystal lattice. Using both the macroscopic and microscopic methods, we have studied magnetic structures, magnetocrystalline anisotropy and magnetization of Fe-rich alloys and intermetallics in multiextreme conditions - under high pressures at low temperatures and in magnetic fields. The observed pressure induced phenomena will be presented and discussed. Specifically we shall consider effects of inequivalent positions and different local neighborhood of Fe atoms in crystal structures and possible anisotropy of magnetic interactions in the Fe-rich alloys and intermetallics.

S1X66 **Functional form of repulsive potential in high-pressure region**

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In our work we have used two different approaches based on the thermodynamic perturbation theory and the molecular light scattering spectra at large shifts of frequencies. The use of a variant of the thermodynamic perturbation theory in which the thermodynamic reference state applied rather than the reference system allowed to establish a connection between of intermolecular potential parameters and thermodynamics properties of a system under this consideration. An analysis of the data for dense gases and liquids reveals the temperature dependence of the steepness parameter for gases and the pressure dependence for liquids. The results obtained on a base of statistical mechanics approach and the molecular light scattering spectra are consistent with each other.

S1Y101 **Many Body Effects on the Transport Properties of Single-Molecule Devices**

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We calculate the electronic transport properties through a molecular device including electron-electron and electron-phonon interactions. The calculations are performed by the Numerical Renormalization Group method. We found that at low temperatures and for weak electron-phonon coupling, the properties of the conductance can be explained in terms of the standard Kondo model with renormalized parameters. At large electron-phonon coupling a charge analog of the Kondo effect takes place. The problem can then be mapped into an anisotropic Kondo model. In this regime the molecule can be strongly polarized by a gate voltage leading to rectification in the current-voltage characteristics of the molecular junction.

S1Y102 **Superlinear Pump Intensity Dependence of Photoluminescence in Si Nanocrystals**

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Recently great attention has been devoted to the search of the optical gain in silicon nanocrystals with the aim of realization of silicon laser. We report on time-resolved measurements ($10^{-11} - 10^{-4}$ s) of photoluminescence (PL) in Si nanocrystals embedded in $SiO_2$ matrix prepared by ion-implantation. PL was excited by picosecond pulses at selected wavelengths at room temperature. For excitation from the certain spectral interval within the absorption edge, we observed a fast (decay time of about 50 ps) PL decay component. The superlinear (quadratic) pump intensity dependence and its spectral position energetically above the pump light (up-converted signal) suggest an important role of a two-photon or a two-step excitation process.

**S1Y103** **Optical studies of radiation effects in bulk and nanoscale $CdS_{1-x}Se_x$ semiconductors**

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Here we report optical studies of MeV-electron irradiated $CdS_{1-x}Se_x$ nanocrystals embedded in a borosilicate glass matrix. Under irradiation the smearing of the confinement-related features in the absorption spectra of the glass-embedded $CdS_{1-x}Se_x$ nanocrystals is observed, accompanied by the absorption edge blue shift. Four possible mechanisms of the observed irradiation-induced absorption edge shift are discussed. The comparison of the obtained results with the measurements for the similar bulk crystals and the host matrix itself have shown the observed effect to be related to the charge-carrier transfer between the nanocrystals and radiation-induced colour centres in the matrix.

**S1Y104** **Magnetization relaxation of single molecule magnets at low temperatures**

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We study the time evolution of systems of magnetic dipoles that relax through quantum tunneling much as $Fe_8$ crystals at very low temperatures. We consider an Ising model of spins with dipolar interactions where a dipole is allowed to flip only if energy change is less than some $\epsilon_w$ [1]. As in experiments we start from partially polarized initial states. Then we apply a magnetic field at $t = 0$, immediately after the system is quenched to very low temperatures. We find that the initial state controls how the system responds later. As in experiments, a hole develops in a magnetic field function. We find that the magnetization varies with $t^p$ while the hole broadens at the same rate. For SC lattices as well as for $Fe_8$, $p \simeq 0.5$, but $p \simeq 0.7$ for FCC and BCC lattices. Still later $m$ levels off to a stationary value controled by the initial state. [1]JJA and JFF, PRL **91** (2003) 047202

**S1Y105** **Quantum measurement in the charge representation**

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We consider counting statistics of charge transfers in a point contact interacting with a quantum system. The main object of the theory is the charge specific density matrix, which allows one to evaluate the probability of the outcome of any joint measurement of the state of the quantum system and the transferred charge. Applying the method of charge projectors, the master equation for the charge specific density matrix is derived using the tunneling Hamiltonian model of the point contact. As an example, the theory is applied to the problem of the von Neumann quantum measurement of a two-state system: The evolution of the charge specific density matrix in the presence of Nyquist or Schottky noise has been studied and the conditions for the realisation of a projective measurement are formulated.

S1Y106 <u>**Phthalocyanines Incorporated into Layered Materials**</u>

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Hydrotalcite layered double hydroxide (LDH) has been studied in this paper for intercalation of two anionic phthalocyanines: zinc(II) 2,9,16,23-tetrasulfo-phthalocyanine (ZnTSPc) and zinc(II) 2,9,16,23-tetra-carboxy-phthalocyanine (ZnTCPc). Out-of-plane twisting by the 5,10,15,20-substituted phenyl rings, provides a route to construct structures extending beyond the macrocycle plane. Layered materials that are able to intercalate neutral or ionic guests into the interlayer spaces offer unique opportunity into this research area. The new systems were prepared by anion-exchange. Powder XRD diffraction data, IR and UV-VIS diffuse reflectance absorption spectra of the intercalated LDH show complete intercalation. Interlayer d-spacing increased from 1.85 nm and 2.27 nm. Could be suggested that the interlayer arrangement is determined by both the layer charge density of the host materials and the position of the anionic groups substituted on the guest molecules.

S1Y107 <u>**Optical response of many-polaron quantum dots**</u>

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The addition energies and the optical absorption spectra are studied for interacting polarons in charged and neutral quantum dots. The path integral formalism for identical particles is used in order to take into account the fermion statistics. The ground-state energy of a confined many-polaron system is analyzed as a function of the number of polarons, of the electron-phonon coupling constant and of the confinement strength. The ground-state transitions between states with different values of the total spin, which occur when varying the confinement energy, are manifested in the optical absorption spectra, in particular, through the dependence of the first frequency moment of the optical absorption spectra on the number of electrons. This work has been supported by the GOA BOF UA 2000, IUAP, FWO-V projects G.0274.01N, G.0435.03, the WOG WO.025.99N (Belgium), eiTT/COBRA, TU/e (The Netherlands) and the European Commission GROWTH Programme, NANOMAT project, contract No. G5RD-CT-2001-00545.

S1Y108 <u>**Magneto-Optical Response by a Layer of Semiconductor Nano-Rings**</u>

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Semiconductor nano-rings (SNR) possess atom-like electronic properties. But unlike quantum dots, SNR can trap a single magnetic flux. This leads to new optical Aharonov-Bohm (AB) effects those occur only in SNR and cannot be observed in quantum dots or metallic meso-scopic rings.
In this theoretical work we predict and disccuss in details a new class of AB effects: AB oscillations of reflectance, transmittance, and absorbance of a layer of InAs/GaAs SNR. We have developed direct expressions for the polarizability within a realistic tree-dimensional model of SNR. This polarizability we use to determine the optical response of a single layer of SNR in magnetic field and to demonstrate AB effects. The effect features suggest that the AB oscillations for a layer of SNR can be measured by means of ellipsometry in low temperature and moderate magnetic fields.

## S1Y109 **Electronic thermal conductivity of disordered metals**

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We investigate the thermal conductivity of interacting electrons in disordered metals [1]. In our analysis we point out that the interaction affects thermal transport through two distinct mechanims, associated with quantum interference corrections and energy exchange of the quasi particles with the electromagnetic environment, respectively. The latter is seen to lead to a violation of the Wiedemann-Franz law. Our theory predicts a strong enhancement of the Lorenz ratio $\kappa/\sigma T$ over the value which is predicted by the Wiedemann-Franz law, when the electrons encounter a large environmental impedance.

[1] R. Raimondi, G. Savona, P. Schwab, and T. Lück, cond-mat/0402245

## S1Y110 **Many Body Effects on the Transport Properties of Single-Molecule Devices**

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The conductance through a molecular device including electron-electron and electron-phonon interactions is calculated using the Numerical Renormalization Group method. At low temperatures and weak electron-phonon coupling the properties of the conductance can be explained in terms of the standard Kondo model with renormalized parameters. At large electron-phonon coupling a charge analog of the Kondo effect takes place that can be mapped into an anisotropic Kondo model. In this regime the molecule is strongly polarized by a gate voltage which leads to rectification in the current-voltage characteristics of the molecular junction

## S1Y111 **First principles simulation of transport properties of metalic nanowires**

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The whole elongation process of different metallic (Al, Au) nanowires has been studied by first-principles total-energy simulations combined with the non-equilibrium Keldysh Green's function approach for electronic transport. As a continuation of our recent work on thin (111) Al nanowires[1,2], where for the first time, we were able to reproduce the characteristic increase in the conductance in the last plateau according to the experiments, we will present large-scale first principles simulation of thick Al wires with different orientations [both (111) and (100)]. We observe the transition from the plastic deformation behavior based on slip planes characteristic of the bulk to the same atomistic processes already identified in the breaking of thin wires. We also have explored the role of different point defects (vacancies and impurities like Si,O,C and H) in the breaking process and the conductance. In all cases we have found dimer-like structures of the nanocontact before final breaking. Finally, we will also discuss the process of the formation of gold monoatomic chains [3] and the role of impurities (H,O) on the whole process and their influence on transport properties. The results will be compared to experimental measurements [4] recently appeared.

[1] P. Jelinek, R. Perez, J. Ortega and F.Flores, Phys. Rev. B 68, 085403(2003).
[2] P. Jelinek, R. Perez, J. Ortega and F.Flores, Surf. Sci., in press (2004).
[3] A.I.Yanson et al, Nature 395, 783 (1998)
[4] A. Halbritter et al, cond-mat/0404171 (2004)

S1Y112 **Thermoelectric transports through charge-density-wave point contact**

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A lot of theoretical and experimental studies of electrical transports through hetero-structures have been done until now. Recent experimental progress also allows measurement of the local thermal currents in small mesoscopic structures. In this study, we investigate thermoelectric properties of a junction with a charge-density-wave (CDW) system. We focus especially on a phase of CDW, and analyze the phase dependence of heat current and electric current in temperature-biased (P)-(I)-(N) junction, where (P) is a conductor with CDW, (I) is an insulator, and (N) is a normal metal. We use the tunnel Hamiltonian and calculate the currents with first-order perturbation theory. Here, we adopt a point contact and assume that the tunnel matrix element doesn't have momentum dependence. Our result shows that heat current doesn't depend on the phase, while electric current driven by temperature difference is proportional to cosine of the phase. This difference can be attributed to particle-hole symmetry and asymmetry of two currents.

S1Y113 **Nonlocal transport in superconductor-ferromagnet hybrid structures**

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We have measured the conductance of nonlocal aluminum-iron spinvalve structures. The sample geometry consists of an aluminum bar with two or more ferromagnetic wires forming diffusive point contacts to the aluminum at varying distances from each other. In the superconducting state, at low temperatures and excitation voltages well below the gap, we observe a spin-dependent non-local conductance. The sign, magnitude and decay length of this signal is consistent with predictions made for crossed Andreev reflections (CAR) in a diffusive superconductor.

S1Y114 **Residual conductance of correlated one-dimensional nanosystems**

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We study a method to determine the residual conductance of a correlated system by means of the ground-state properties of a large ring composed of the system itself and a long non-interacting lead. The transmission probability through the interacting region, and thus its residual conductance, is deduced from the persistent current induced by a flux threading the ring. DMRG techniques are employed to obtain numerical results for one-dimensional systems of interacting spinless fermions at arbitrary filling. As the flux dependence of the persistent current for such a system demonstrates, the interacting system coupled to an infinite non-interacting lead behaves as a non-interacting scatterer, but with an interaction-dependent elastic transmission coefficient. Among the applications discussed are systems where both, interaction and disorder are relevant.
Phys. Rev. B 67, 235306 (2003); arXiv:cond-mat/0402250

**S1Y115**   **Role of surface anisotropy for magnetic impurities in electron dephasing and energy relaxation**

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There is a serious puzzle concerning the concentration of magnetic impurities estimated from electron dephasing (MSU) and energy relaxation experiments (Saclay) in mesoscopic metallic samples. The dephasing rate was determined from magnetoresistance while the energy relaxation from nonequilibrium transport on mesoscopic scale. The estimated magnetic impurity concentrations even can deviate by more than hundred. The surface anisotropy due to the spin-orbit coupling in the host was suggested to explain the size dependence of the Kondo effect. At low temperature the spin is blocked and therefore cannot contribute to the dephasing, in contrary to mesoscopic transport experiments. There, the applied voltage and therefore the smearing of the energy distribution is usually larger than the anisotropy, thus the spin can move and induce the energy relaxation. The theory and the experiments are compared for integer and half-integer spins.

**S1Y116**   **Spin-dependent transport through quantum dots in the cotunneling regime**

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The first and second order spin-dependent transport through quantum dots is analyzed theoretically using the real-time diagrammatic technique. It is shown that in the parallel configuration of the leads' magnetic moments the second-order processes lead to an effective spin-splitting of the dot level at low bias voltage. Furthermore, a strong parity effect for the linear-response TMR is found in the cotunneling regime. In addition, a zero-bias anomaly in the differential conductance for anti-parallel configuration is predicted. The anomaly manifests itself as a maximum in differential conductance and results from spin asymmetry between cotunneling events and competition between the one-barrier and two-barrier second-order tunneling processes.

**S1Y117**   **Effects of pumping in a quantum wire**

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We discuss charge and spin pumping in an interacting one-dimensional wire, modelled by a Luttinger liquid. We show that a spatially periodic potential modulated in space and time acts as a quantum pump inducing a dc current component at zero bias. The current generated by the pump has a power law dependence on the frequency or temperature with the exponent determined by the interaction in the wire, while the coupling to the pump affects the amplitudes only. We also show that pure spin-pumping can be achieved, without the presence of a magnetic field or in absence of spin-orbit interaction. Finally, we study the noise spectrum which shows singularity at a finite frequency due to charge and spin pumping. We present a possible experimental device for the pumping.

**S1Y118** **Why the dc power source can be observed under equilibrium conditions.**

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The observation of the quantum oscillations of the dc potential difference on segments of asymmetric superconducting loops [1] demonstrates that the persistent current behaves totally as conventional current. Therefore the observation of the persistent current at non-zero resistance under equilibrium conditions [2] is experimental evidence of a persistent power, i.e. a dc power source observed in the equilibrium state. It is explained in the present work why the persistent power can be observed in quantum systems.

[1] S.V.Dubonos et al. JETP Lett. 77, 371, (2003); cond-mat/0303538.
[2] A.V. Nikulov, Phys.Rev.B 64, 012505 (2001).

**S1Y119** **Double Quantum Dots out of Equilibrium**

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A new mechanism of resonance Kondo tunneling through a parallel double quantum dot in T-shaped geometry is proposed [1]. It is shown that a non-equilibrium Kondo resonance in a double dot with even occupation and singlet ground state is induced by external voltage applied to the leads. Using new fermionization procedure for SO(N) groups [2] and the renormalization group technique we derive the scaling equations and calculate the differential conductance as a function of auxiliary dc- and ac- bias. We analyze the decoherence effects associated with the triplet/singlet relaxation and discuss the shape of differential conductance as a function of a dc-bias and temperature.

[1]. M.Kiselev, K.Kikoin and L.W.Molenkamp, Phys. Rev. B 68, 155323 (2003)
[2]. M.Kiselev and R.Oppermann, Phys.Rev.Lett. 85, 5631 (2000)

**S1Y120** **Current and noise in a model of an AC-STM molecule-metal junction**

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The transport properties of a simple model for a finite level structure (a molecule or a dot) connected to metal electrodes in an alternating current scanning tunneling microscope (AC-STM) configuration is studied. The finite level structure is assumed to have strong binding properties with the metallic substrate, and the bias between the STM tip and the hybrid metal-molecule interface has both an AC and a DC component. The finite frequency current response and the zero frequency photo-assisted shot noise are computed, and examples for a single site molecule and for a two-site molecule are examined.The zero frequency photo-assisted shot noise serves as a useful diagnosis for analyzing the energy level structure of the molecule. The present work motivates the need for further analysis of current fluctuations in electronic molecular transport.

S1Y121 **Semiclassical evaluation of quantum fidelity**

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Quantum fidelity (Loschmidt echo) measures the sensitivity of quantum motion to perturbations, and the simplest experimental realization is the NMR spin echo. We present a numerically feasible semi-classical (SC) method to evaluate quantum fidelity in a classically chaotic system. It was thought that such SC evaluation would be intractable, but instead we show that a uniform SC expression not only is tractable but it gives remarkably accurate numerical results for the standard map in both the Fermi-golden-rule and Lyapunov regimes. Because it allows Monte Carlo evaluation, the uniform expression is accurate at times when there are $10^{70}$ semiclassical contributions. Remarkably, it also explicitly contains the "building blocks" of analytical theories of recent literature, and thus permits a direct test of the approximations made by other authors in these regimes, rather than an a posteriori comparison with numerical results. We explain in more detail the extended validity of the classical perturbation approximation (CPA) and show that within this approximation, the so-called "diagonal approximation" is automatic and does not require ensemble averaging over realizations of a disordered potential.

S1Y122 **Phonon-induced Decoherence of Andreev Levels in Superconducting Junctions**

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We investigate decoherence of superconducting bound states lying deep within the superconducting energy gap and interacting with acoustic phonons. The phonons present potential source of intrinsic qubit decoherence additional to the extrinsic decoherence due to environmental noise and fluctuations in biasing circuits. We derived kinetic equation for the density matrix of Andreev two-level system by using a path integral technique, and show that the kinetic equation has a non-linear form and leads to significant slowdown of the decoherence process at temperature smaller than the level spacing. The reason is the fermionic nature of the Andreev levels: the levels are not isolated from the continuum quasiparticle states, the total level population fluctuates, and the Pauli exclusion principle suppresses the interlevel transitions. (A. Zazunov et al., cond-mat/0404656)

S1Y123 **Strain and interdiffusion in lateral InAs quantum dot molecules**

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Lateral quantum dot molecules are ordered arrangements of several quantum dots placed one near the other. For InGaAs and InAs on GaAs(100), it has been shown that they can be produced by molecular beam epitaxy exploiting a self-organization process: the quantum dots nucleate preferentially around nanoholes in the substrate. We have performed a systematic study of different growth stages of InAs quantum dot molecules using grazing incidence x-ray diffraction (GID) in combination with anomalous scattering. These experiments give information about shape, strain, and interdiffusion at the different growth stages. Here, we focus on the initial hole formation by in situ etching methods, and on the comparison between strain and interdiffusion in the quantum dot molecules and conventionally grown quantum dots.

S1Y124 **Tomonaga-Luttinger Scaling of Charge Fluctuations in a Nanoscale Structure**

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We propose an experiment to study electron correlations in a one-dimensional nanostructure, avoiding the usual complications associated with transport measurements. The setup consists of a quantum box, biased by a gate voltage, and side-coupled to a quantum wire by a point contact. Close to the degeneracy points of the Coulomb blockaded box, and in the presence of a magnetic field sufficiently strong to spin polarize the electrons, the setup can be described as a Tomonaga-Luttinger liquid interacting with an effective Kondo impurity. Using exact nonperturbative techniques we predict that the differential capacitance of the box will exhibit distinctive Tomonaga-Luttinger scaling with temperature and gate voltage. By turning off the magnetic field the spins of the electrons open up an additional channel for interactions. We conjecture that for this case the system can be mapped onto the two-channel Kondo effect in a spinful Tomonaga-Luttinger liquid.

S1Y125 **Non-gibbsian stationary-state electronic distribution in quantum dots**

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Electron-LO-phonon system of semiconductor quantum dot is shown to display a non-gibbsian electronic distribution in steady state. The effect is ascribed to multiple electronic scattering on LO phonons in quantum dot. Theoretical results are compared with recent experiments on electronic up-conversion. Simple derivation of corresponding transport equation is given and role of this equation in determination of thermodynamic properties of quantum dots is discussed.

S1Y126 **Effect of internal bias field on 180 degree domain switching in inhomogeneous alkylammonium halogenobismuthate crystal**

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Depolarization process, which causes a reduction of the stored voltage signals is one of the impediments, limiting the usage of the ferroelectric materials in the memory devices. In this report the characteristics of switching and depolarization (backswitching) processes were presented for inhomogeneous alkylammonium halogenobismuthate crystal. The presence of the internal bias field in these crystals gives rise to an axial anisotropy of the coercive field, resulting in spontaneous backswitching upon removing of the external field. This effect was investigated by direct observation of the domain structure (by nematic liquid crystal decoration technique) and by switching current registration in the high electric field ranges. The presented results show that a strong correlation exists between internal bias field and the domain stabilization mechanism. The experimental results were analyzed in the framework of Avrami classical model of nucleation.

### S1Y127 Thermo-responsive PNIPAM Encapsulated in Polymeric Microcapsules

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The layer-by-layer assembly (LBL) of polyelectrolytes has been extensively studied for the preparation of capsules due to the versatility of the build-up process, and because of their possible use as microcontainers. Capsules loaded with a thermo-sensitive species could be used as stimuli-sensors. Encapsulated polymers could also act as adsorbents for substrates or as substrates themselves and could be used for chemical reactions inside the capsules that will thus be employed as microreactors or as drug delivery systems. We present two methods of encapsulation that reproducibly yield PNIPAM fill polymeric capsules. The presence of poly-NIPAM only inside the LBL fabricated capsules has been confirmed with Raman confocal microscopy, confocal microscopy, AFM, and SEM. With these techniques it has also been shown the PNIPAM inside the capsule maintains its thermo-responsive properties

### S1Y128 Collective Dynamics of an Incommensurate MnSi$_x$ Composite

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A still fundamental pending question in aperiodic composites concerns the nature of the collective modes. The incommensurate structure is constructed from two or more interpenetrating sublattices with different periodicities in at least one crystallographic direction. The question of the lattice dynamics offering complex possibilities, is still needing elucidation. Specific low-frequency excitations are expected due to the inter-lattices coupling. Such systems may exhibit a particular acoustic-like phonon called sliding mode, resulting from the infinite degeneracy of the ground state versus the relative positions of the sublattices. This problem is addressed by a neutron scattering analysis of the so-called higher manganese silicide MnSi$_x$, well known for thermoelectric applications.

### S1Y129 MONTE CARLO STUDY OF AQUEOUS SOLUTION OF ETHANOL

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Monte Carlo calculation results for pure liquid ethanol and water-ethanol solutions calculated in the isothermal and isobaric ensemble at T=300K are presented. The analysis of hydrogen bounding, energetics between ethanol molecules and water molecules at different molar concentrations of ethanol was done. Radial distribution functions of type water-ethanol have characteristic features at xet 0.22 and at xet 0.75.

## S1Y130 **Various physical properties of liquid transition metals**

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A pseudopotential model depending on an effective core radius but otherwise parameter free is used [1-3] to study structure factor, radial distribution function, longitudinal and transverse phonon frequencies, elastic constants, bulk modulus, longitudinal and transverse velocities, Debye temperature, autocorrelation function, characteristic frequencies, viscosity coefficient and surface tension of liquid Cu, Ag, Au, Ni, Pd, Pt, Rh and Ir at and above melting point temperatures. Fourier transforming the structure factor, which is derived from a charged hard-sphere model approximation, obtains the radial distribution function. The beauty of this approximation is that it needs pseudopotential form factor for the calculation of structure factor. So this gives the better explanation of structure factor than any other approximations. The contribution of d-like electrons is taken into account by introducing a repulsive short-range Born-Mayer term. A good agreement between theoretical calculations and experimental findings has confirmed the ability of this [1-3] model potential for predicting the structure dependent properties of liquid transition metals.
References:

[1] J. K. Baria, A. R. Jani, Physica B 328, 317 (2003).
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[3] J. K. Baria, A. R. Jani, Pramana J. of Phys. 60, 1235 (2003).

## S1Y131 **Structure and physical properties of sodium malate dihydrate**

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In this work, the structure of Sodium Hydrogen Malate Dihydrate, $NaH(C_4H_4O_5).2H_2O$, has been determined at room temperature using X-ray diffraction techniques. The space group is monoclinic $P2_1$ with lattice parameters a= $7.286\AA$, b= $7.357\AA$, c= $7.667\AA$ and $\beta$= $110.99\AA$. Some of its physical properties have been studied. The compound shows a phase transition at about 325K that has been identified by Differential Scanning Calorimetry and dielectric measurements performed on polycrystalline samples. Preliminary measurements indicate that the second harmonic generation efficiency at a fundamental wavelength of 1064nm is roughly the same as KDP. We acknowledge financial support of the Spanish CYCIT project BFM2002- 03327 as well as FEDER funds.

## S1Y132 **X-ray Diffraction Measurements of Slightly Stressed Titanium Nitride Thin Films**

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Thin polycrystalline layers plays substantial role in many of technical applications nowadays. The aim of our study was sintered tungsten carbide material coated with thin layers of TiN, prepared by CVD method. Such materials are extensively used as different kinds of drills and cutting tools because of its specific mechanical, physical and chemical qualities. One of the principal parameter, which reflects in mechanical properties, is presence and magnitude of residual stress. The samples were characterized using the x-ray diffraction, which is method appropriate for thin layers investigation. Current work discusses and compares different techniques that are commonly used for x-ray diffraction stress measurements. The residual stress calculations were performed using both - methods based on the diffraction elastic constants and mechanical elastic constants as well. We also discuss various grain interaction models (Reuss, Voigt and Neerfeld-Hill) and its influence on calculated results.

**S1Y133** **Microstructural aspects on the processing of Fe-Si alloys studied by Mossbauer spectroscopy and positron annihilation techniques**

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Although the best compromise for the magnetic properties of high-Si steel is obtained around 6.5 wt.%Si, the processing into a thin sheet remains challenging for higher concentrations than 3.5 wt.%Si due to its poor cold ductility. Ordering enhancement has been generally identified as the reason for this lack of workability. However, defects may have a role too on the large change of the mechanical properties. Mossbauer spectroscopy has been used to characterize the order present in several alloys with Si-contents up to 11.7 wt.% and different thermomechanical treatments. Positron annihilation experiments have detected an equilibration process for the defects occurring at room temperature. The movement of interstitial atoms nearby the defects might be the reason for this behaviour.

**S1Y134** **Synchrotron Radiation Renninger Scan in the study of Temperature induced Rochelle Salt Phase Transition**

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X-ray Renninger scan (RS) using synchrotron radiation to study temperature induced phase transition in Rochelle salt crystal is discussed. RS ($\phi$-scan) provides 3D lattice information (interaction between planes with several orientations within the crystal) and enough sensitivity to detect subtle unit cell distortions when submitted to external stimulus (symmetry changes), temperature in this case. Between 255K and 297K($T_c$), Rochelle salt is ferroelectric, monoclinic symmetry ($P2_11$). Out of this range, it is paraelectric, orthorhombic ($P2_12_12$). RS were performed in the Brazilian National Synchrotron Laboratory (LNLS) using ($\mathbf{10}00$) Rochelle salt weak reflection from 260K up to 331K. The expected structural phase transition was clearly observed in these measurements and also in the RS simulation through two typical 4-beam cases:$(000)(\mathbf{10}00)(913)(113)$ peak shift and $(000)(\mathbf{10}00)(81\bar{2})(21\bar{2})$ peak splitting.

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**S1Y135** **Small Angle Neutron Scattering in mesoscopic studies of patterned media**

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Self-assembled and patterned magnetic nanostructures are currently the subject of much interest due to both its high potential for future nanotechnology and its interesting magnetic properties. Microscopic characterisation of patterned media is essential for the understanding of the local magnetic properties of these systems. In our studies of nanoscopic magnetic arrays we are looking at the possibility of using Small Angle Neutron Scattering (SANS) for investigation of the local magnetic density of the individual elements comprising the medium. In this contribution we will present results from our first SANS experiments on Co based nanomagnetic arrays and demonstrate the advantages in application of the neutron scattering techniques to magnetic patterned structures.

**S1Y136** **The resolution function for a pulsed-source TOF neutron spectrometer with mechanical monochromator**

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The concept of resolution function has been first introduced by Nathans and Cooper in 1967. The proposed computational method,is suited only for rather simple configurations as the conventional double and triple axis spectrometers are.The matrix procedure first proposed by A.D.Stoica in 1975 is suited for a large variety of experimental configurations, in particular for sophisticated ones using the focusing effects where spatial effects are important, or for TOF instruments. The Monte Carlo procedure requires computers with increased memory and computing speed while, for the matrix method, a normal 486 PC is quite suited, with computing times of 1-2-seconds. Therefore the matrix method should be preferred. If a precise description of the line profile is needed, the M.C. procedure should be used. The general theory for the matrix method is briefly given. The application of this method for a pulsed-source TOF neutron spectrometer with mechanical monochromator is then given.

**S1Y137** **Dynamic Characteristics of Cubic Molecular Crystals with Noncentral Interaction**

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The effect of the noncentral interaction with the nearest neighbors upon the dynamic characteristics of cubic crystals has been considered. In body-centered (BCC) and simple cubic lattices the noncentral interaction affects the character of dispersion relations qualitatively, but in face-centered (FCC) crystals it causes only quantitative changes. It is shown, that in FCC crystals even the relatively weak noncentral interaction influences essentially the dynamic characteristics, in particular the elastic moduli and the frequencies of transverse vibrations along the [110], [111] directions. Numerical estimation was performed for FCC and BCC cryocrystals. The force constants have been calculated for $C_{60}$, $CH_4$, $CD_4$, $CO$, $CO_2$, $N_2$ and $SF_6$.

**S1Y138** **COMPUTER PROGRAM TO DESIGN CRYSTAL NEUTRON DIFFRACTOMETERS CONFIGURATIONS AND TO EVALUATE THEIR RESOLUTION AND LUMINOSITY PERFORMANCES**

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The DAX program allows for the resolution function, line widths and intensities computations for a two-axis neutron spectrometer. Both the configurations with one or two crystals monochromator group, with plane (the conventional case) or curved crystals (the focusing case) with or without Soller collimators, diaphragms or neutron guide are allowed for. The computational method used is the matrix one.The experimental configuration optimization can be made either analytically, using the corresponding optimizations conditions or numerically, by minimizing the optimization parameter. The focusing conditions for an ideal configuration, to be used in a numerical optimization procedure as 0-th order approximation, is given. A library with the relevant data concerning the most used crystals is included in the program.

**S1Y139** **Elastic properties of submicrocrystalline aluminium alloys**

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High-pressure technique was applied to produce submicrocrystalline materials by severe plastic deformation. The materials were initially processed by cold or hot hydrostatic extrusion and then deformed at room temperature under the high hydrostatic pressure conditions to avoid microcracking. This process was controlled with an acoustic emission method. Due to the high-pressure conditions a submicrocrystalline structure was achieved both for a dispersion-strengthen aluminium alloy and for a britlle at room temperature intermetallic NiAl. The grain size of the material was controlled using TEM. A full tensor of elasticity of obtained fine-grained and textured materials was determined with a resonant ultrasound spectroscopy (RUS) method based on measuring the spectrum of the mechanical resonances of a small sample. Equivalent elastic moduli of the isotropic material were calculated using the Voight-Reuss-Hill averaging method for measured elastic constants. They were compared with the values obtained for coarse-grained polycrystals of these materials measured with the RUS and classical pulse-echo Papadakis methods. The differences between the elastic moduli of the fine-grained materials and the coarse-grained ones are interpreted as an effect of the microstructure defects resulting from the small size of submicrocrystalline materials.

**S1Y140** **Peculiarities of the phonon spectra derived from specific heat measurements for titanium dihalcogenide based compounds**

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The specific heat study has been performed for quasi-two dimensional compounds $MyTiX2$ (X=Se, Tl) intercalated by M = Ag, Ni. Using the Mobius inverse theorem the phonon density of states (PhDOS) in a low frequency region has been calculated from specific heat data. The Ag-intercalation in $TiSe2$ at y= 0.25 increases the PhDOS twice as much in comparison with the parent compound that means a precursor of soft lattice mode. An insertion of Ni atoms depletes the low frequency part of PhDOS that agrees with the stiffening of the lattice along c-axis.

**S1Y141** **Reconstruction of Atomic Dynamics and Thermodynamics of Face-Centred Cubic Crystals from Elastic Moduli**

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In this study the elastic moduli data were used to construct the atomic dynamics and thermodynamics of solid heavy inert gases and face-centred cubic metals. It is shown, that the lattice vibrations of Ar, Kr and Xe, as well as Ag, Cu, Pb, and Al can be described correctly taking into account only the nearest-neighbour interaction .To put it differently, the atomic dynamics of these substances can be restored completely from their elastic moduli. For some metals, such as Au, Pd and so on, it is necessary to allow for the next-nearest neighbour interaction. The information about this interaction can be derived, for example, from the highest frequencies of different- polarisation waves propagating in the crystal.

## S1Y142 **Specific heat of TbMn$_2$(HD)$_x$**

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Specific heat SH) measurements of TbMn$_2$(HD)$_x$ (x = 0, 3) powders have been performed in the temperature range from 2 K to 350 K and in the magnetic field of 0 and 9 T in the PPMS by a relaxation method. For the pure sample (x=0) the anti-ferromagnetic phase transition was revealed by a single SH peak at temperature of 45 K (T$_N$), whereas a double SH peak respectively at 275 K and 280 K and an upturn below 3 K were observed for the hydride one (x=3). Under the applied magnetic field of 9 T, the SH upturn was suppressed, whereas no visible influence on the double peak was found.

## S1Y143 **Crystal structure of A-site deficient La$_4$Mg$_3$W$_3$O$_{18}$ layered perovskite**

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The crystal structure of A-site deficient La$_4$Mg$_3$W$_3$O$_{18}$ oxide has been solved by X-ray powder diffraction in combination with group theoretical analysis. At high temperature, above 700 K, the crystal structure is orthorhombic (space group Ibam, $2a_p \times 4a_p \times 2a_p$) and represents a sequence of [LaO]-[Mg$_{1/2}$W$_{1/2}$O$_2$]-[La$_{1/3}$O] layers stacked along the b axis. The lanthanum ions and vacancies in the [La$_{1/3}$O] layers are ordered and form rows along the c axis. The ordering of vacancies in the lanthanum poor layers is connected with the ionic ordering between Mg$^{2+}$ and W$^{6+}$ in the neighbour [Mg$_{1/2}$W$_{1/2}$O$_2$] blocks. Around 700 K, due to an anti-phase octahedral tilting, a continuous phase transformation mediated by the $\Gamma_2^+$ irreducible representation, from orthorhombic (Ibam a$^0$b$^0$c$^0$) to monoclinic (C2/m a$^0$b$^0$c$^-$) symmetry, takes place.

## S1Y144 **Crystalline orientations and electrical conductivity of tin oxide and zinc oxide thin films**

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In this paper, we present results on electrical resistivity of zinc oxide thin films deposited by spray and of both undoped and antimony-doped tin oxide thin films deposited by chemical vapour deposition (CVD). We will first present the experimental procedure, dispositif used and sample preparation than the results will be follow and finally the discussion and conclusion drawn from those experimental results will be summarised. The deposition and post-deposition parameters are known to affect strongly the film structure and electrical resistivity. We have investigated the influence of film thickness and thermal annealing on structural and electrical properties of the films. The structure was analysed by X-ray diffraction. We observed a variation of grain size and crystalline orientation. The electrical properties varied with grain size and thermal annealing under air or vacuum .

**S1Y145** **Lattice vibrations in PZN:8PT single crystal**

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A complex perovskite solid solution with 72% of $Pb(Zn_{1/3}Nb_{2/3})O_3$ and 8% of $PbTiO_3$ (PZN:8PT) has triggered enormous interest in the past decade due to its record piezoelectric properties (in a single-crystal state). We will present infrared and Raman spectra of this material measured in an identical single crystal sample in a broad temperature interval (10-500 K). In contrast to the case of a close model relaxor system $Pb(Mg_{1/3}Nb_{2/3})O_3$ (PMN), none of the observed optic modes in PZN:8PT showed pronounced frequency softening with temperature. We compare various approaches to identifying of optic modes in mixed perovskite systems and propose a complete assignment of the observed spectral lines of PZN:8PT.

**S1Y146** **A dodecagonal structure constructed by projection in two stages**

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Dodecagonal and octagonal quasicrystalline structures are known in several alloy systems. They are quasiperiodic in a plane and periodic in its perpendicular direction. Physical quasicrystals are routinely represented as projections of periodic structures in higher dimensions. It is therefore interesting to study intermediate structures obtained by projection from $D(> 3)$ dimensions onto 3D so that a second projection be quasiperiodic in 2D. This has been achieved for octagonal and partly for dodecagonal quasicrystals. Here I present an intermediate structure obtained projecting onto 3D the 4D (body and face) centered cubic lattice. The unit cell is a 24-cell; being self-dual it is also the Voronoi domain. Yet the respective 3D projections are different. The second projection onto 2D yields the desired structure quasiperiodic in a plane and periodic in its perpendicular.

**S1Y147** **Morphometry of condensed matter:**
**physics and geometry of spatially complex structures**

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Spatially complex disordered matter such as foams, gels and porous media are of increasing technological importance due to their shape-dependent material properties. But the shape of disordered structures is a remarkably incoherent concept and cannot be captured by correlation functions alone which were almost a synonym for structural analysis in Statistical Physics since the very first X-ray scattering experiments. However, in the last 20 years numerous methods such as AFM and computer tomography have been developed which allow quantitative measurements of complex structures directly in real space. Integral geometry furnishes a suitable family of morphological descriptors, known as Minkowski functionals, which are related to curvature integrals and do not only characterize connectivity (topology) but also size and shape of disordered structures. Furthermore, Minkowski functionals are related to the spectrum of the Laplace operator, so that structure-property relations can be derived for complex materials. Percolation thresholds and fluid flow in porous media, for instance, can be predicted by measuring the Minkowski functionals of the pore space alone. Also, evidence was found in hard sphere fluids that the shape dependence of thermodynamic potentials in finite systems can be expressed solely in terms of Minkowski functionals. Finally, a density functional theory is constructed on the basis of Minkowski functionals which allows an accurate calculation of correlation functions and phase behavior of mesoscopic complex fluids such as microemulsions and colloids.

**S1Z201** **Eigenmodes of electromagnetic fields in the presence of a magnetic domain structure**

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At low temperatures the quantum oscillatory part of the magnetic susceptibility $\chi$ of metal placed in quantizing magnetic field, can reach values of the order of unity. We have investigated the low-frequency weakly damped eigenmodes of the electromagnetic field in the nonferromagnetic metals, under the conditions, when $\chi > 1/4\pi$ and the sample breaks into alternating domains with different values of a magnetic induction. In the case, when the waves propagate along an external magnetic field the frequency of a wave coincides with helicon frequency in classically strong magnetic fields. At an arbitrary direction of propagation of the wave the non-stationary magnetic field can be presented as a functional series, with factors satisfied the infinite system of the linear equations. We have defined the spectrum of the waves from the conditions of solvability of this system.

**S1Z202** **Electronic Properties of Curved Surfaces: Quantum Effects Induced by Curvature, Symmetry and Connectivity**

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Meso-porous materials are characterized by the porosity and periodicity in nanometer scale. The surfaces of the pores often constitute exotic curved surfaces, which when used as propagating media for electronic wave functions can exhibit new quantum effects induced by the geometrical properties. Here we present a preliminary theoretical investigation on the electronic properties of metallic curved surfaces using an approach of a single electron Schrödinger equation in which the electron is strongly constrained onto the surfaces. In particular, we will concentrate on the quantum effects induced by the curvatures, symmetry and connectivity. We discuss the following two different problems: (1) Electronic structures of triply periodic minimal surfaces, especially those of G-surface, (2) The effects of magnetic fields on the electronic properties of curved surfaces.

**S1Z203** **ENERGIES OF FORMATION OF SIGMA PHASE IN Mo-BASED SYSTEMS**

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In systems Mo-Co, Mo-Cr and Mo-Fe, we performed total energy calculations of all 32 possible configurations of sigma phase using the LMTO-ASA method. The energy differences between the sigma phase and the Standard Element Reference (SER) state were investigated by means of the FLAPW method using the GGA approximation for the exchange-correlation energy. The optimisation of the lattice parameters of all structures was included. The combination of LMTO and FLAPW results yields the positive energies of formation of sigma phase with respect to the weighted average of total energies of SER. Comparison of calculated energies of formation of sigma phase with results of CALPHAD approach is shown. It is supposed that the experimental stability of the Mo-Fe and Mo-Co sigma phases is due to configurational and vibrational entropies.

**S1Z204** **About the high frequency properties of layered conductive film**

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The propagation of a monochromatic longitudinal acoustic wave along the weak conductivity axis of a thin quasi-two-dimensional conductive film, in an absence of external magnetic field, is studied theoretically. It is shown that under certain conditions, the formation of standing ordinary (OAW)and anomalous (AAW) acoustic waves is possible. The frequency dependence of the amplitudes of both waves has been derived, as well as the mean acoustic energy. For certain values of the characteristic parameters the AAW in the film may be dominant. From the resonance conditions for formation of standing OAWs and AAWs (especially AAW) it is possible to obtain information about the electronic structure of the quasi-two-dimensional conductors, e.g. the corrugation parameter $\eta$ or the relaxation properties of the charge carriers.

**S1Z205** **Influence of pressure on physical properties of $Sn_2P_2S_6$ and $SnP_2S_6$ crystals: *ab initio* investigations**

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Using the density functional theory in the local density approximation the pressure dependences of the crystal structure, dynamical and electronic properties of the $SnP_2S_6$ layered semiconductor and $Sn_2P_2S_6$ proper ferroelectric under pressure have been theoretically investigated. Theoretically obtained long-wave phonon frequencies for this compounds are in excellent agreement with known experimental frequencies. The equation of state for both phases of $Sn_2P_2S_6$ and layered $SnP_2S_6$ crystals has been thoroughly investigated. The suggestion of the first order phase transition of $Sn_2P_2S_6$ at 0.6 GPa hydrostatic pressure and of the existence of the modulated structure in the range of 0.6-1.2 GPa has been made. The band structure of $SnP_2S_6$ have been investigated. At the pressure of above 10 GPa the indirect-direct band gap crossover is observed.

**S1Z206** **Optimization of Analytical Expression for Power Losses in Soft Magnetic Materials by Feed Forward Neural Network and Genetic Algorithm**

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A mathematical model for core losses was improved for frequency and geometrical effects using experimental data obtained from toroidal wound cores. The improved mathematical model was applied to the other soft magnetic materials and optimizes its parameters with the aim of neural networks. A 6-neuron input layer, 9-neuron output layer model with two hidden layers were developed. While the input parameters were outer and inner diameters, strip width, magnetising frequency, magnetic induction and the measured power loss, the output parameters were correlation coefficients and the power loss obtained from mathematical model. The network has been trained by the genetic algorithm. When the network was tested, the linear correlation coefficient was found to be 99%.

## S1Z207 **Monomers for Discotic Crystals**

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Derivatives of 1,3,5-trispyrazolylbenzene (TPB) have been studied by density-functional and semi-empirical methods to assess their potential as building blocks for discotic liquid crystals. Structural and vibrational data provide evidence that TPB derivatives exibit properties which favour the desired columnar stacking and allow the tuning of the side chains. The molecules are planar three-fold symmetric. According to a vibrational analysis all investigated molecules exhibit sufficient rigidity for columnar stacking. Yet, they are also flexible enough in order to tolerate small deformations which may occur as packing effects. The dipole moments of the most stable conformers are directed perpendicular to the molecular plane, thus they favour the stacking to three-fold symmetric columns.

## S1Z208 **Chiral currents in the Quantum Hall Effect.**

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The conductive channels and the current distributions in a two-dimensional electron gas in magnetic fields are studied using the Keldysh nonequilibrium Green's function formalism, and a site representation of the electron Hamiltonian. First, we consider an infinite two-dimensional Hall bar, with longitudinal translation symmetry, and provide the microscopic picture of the edge conductive channels, and their conductance quantization.
Then we superimpose to the ideal substrate different model potentials, and focus on the peculiar imperfections of the sample that do not change the total net current through the device. In general, these obstacles have a strong influence on the local currents broadening the spatial extension of conductive channels and stabilizing the Fermi energy between Landau levels.
By means of analytic elaborations and detailed numerical results, we show that the value of chemical potentials at the edges and quantization of the Hall conductance are exact universal features of the conductive channels.

## S1Z209 **THERMOELECTRIC PHENOMENA IN LAYERED CONDUCTORS IN MAGNETIC FIELD**

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The dependence of the thermoelectric force in layered conductors with quasi-two-dimensional electron energy spectrum of arbitrary form versus the magnetic field has been theoretically investigated. It is shown that the dependence of the thermoelectric force on the magnitude and the orientation of the magnetic field with respect to the layers contain detail information for the distribution of the charge carriers velocities on the Fermi surface.

S1Z210  **Phase Formation at Metal-Semiconductor Interfaces**

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The preparation of structurally and electronically well-defined interfaces between metallic Ti and semi-conducting Si is complicated by the formation of crystalline and amorphous binary compounds with a wide compositional range. Molecular-dynamics density-functional calculations are carried out for the prototype interface Ti(0001)—Si(111), where $Ti_5Si_3$, TiSi, and $TiSi_2$ phases were observed experimentally. In accordance with those results, the first steps of the compound formation show that an amorphous film is accessible at temperatures, for which the crystalline binary compounds do not yet exhibit melting. The interface reaction is accompanied by an equilibration and reduction of the stress tensor components, present in the atomically flat interface due to the lattice mismatch between Si(111) and Ti(0001). Thus, the silicide formation is not only driven by the electronegativity difference of Ti and Si, but enhanced by an elastic contribution.

S1Z211  **Cobalt doping of Anatase Thin Films**

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About two years ago Co-doped $TiO_2$ anatase has been discovered to exhibit ferromagnetism at and above room temperature, i.e. to be a magnetically robust diluted magnetic semiconductor (DMS). Since then it has attracted considerable interest, but there is still controversy over the origin of the magnetism as well as the influencing factors.
In this work a low-energy $\Sigma$ 5(113)[-110] grain boundary in anatase is studied by density functional band structure calculations employing norm-conserving pseudopotentials and plane waves. The interfacial structure in pure anatase exhibits close structural and electronic similarity to the pure bulk anatase crystal. Yet, the grain boundary acts as a sink for dopant atoms, such as Co. This result confirms the importance of the investigation of grain boundaries in the discussion of DMS' properties.

S1Z212  **Finite-Size Effects in Alloyed Nanowires**

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Density-functional band-structure calculations were carried out for two-shell metallic nanowires from Au and from AgAu and PdAu alloys. All structures are local minima of the formation energy and more stable than the planar Au(111) surface. The stability of the most favourable structure increases in the order $PdAu_8 < Au_9 < AgAu_8$. This trend coincides with the tensile stress acting on the central monatomic chain. An analysis of the electronic structure shows that the binding between the two shells is not strongly directional. Yet, the interatomic interaction along the central chain is weakened compared to the interaction in the monatomic wire, thus the tensile stress along this direction is alleviated. In $Au_9$ and $AgAu_8$ the central conductance channel is depopulated, in $PdAu_8$ not. These findings rationalise the lower conductivity of PdAu nanocontacts compared with AgAu contacts obtained recently by break junction experiments. [1] www.abinit.org

**S1Z213** **Local vibrations of impurities near microcontacts and vacancies**

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The expressions for conditions when local vibrations (LVs) exist and for their frequencies, intensities, and amplitudes of damping with distance from defect are obtained in the case when impurities are located near microcontact i.e. on various crystal surfaces as well as on different ribs and apexes formed bycrossing of the surfaces. LVs are demonstrated [1] to be due to by the nearest neighbours of impurity essentially. Therefore, noticeably differ LVs for displacement of impurity only along the longitudinal or transverse directions with respect to surface of the crystal, along and normal to the ribs. Properties of LVs caused by isotopic impurity in vicinity of vacancy or group of vacancies are analysed as well.

1. O.V. Kotlyar, S.B. Feodosyev, 19th General Conference of CMD, Europhysics Conference Abstract, V. 26A, C22.P.3.7 (2002)

**S1Z214** **Multiscale Investigation of Ferroic Multilayers**

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Highly mobile charge carriers have recently been reported for the interface $LaAlO_3(001)|$ $SrTiO_3$. This effect was attributed to the presence of free electrons at the formally negatively charged $AlO_2{}^-$ termination layer, whereas the positive charge carriers of the alternative $LaO^+$ termination is localised. DFT investigations confirm that negative charges of an $AlO_2{}^-$ termination occupy spatially extended electronic states, whereas the positive charges at the $LaO^+$ termination are localised. However, an analysis of the band structure and the density of electronic states suggests that the observed metallic properties are only achievable if only a smaller fraction of the formal charge is present at the interface. With the help of mesoscopic modelling the electron (de)localisation is studied as a function of the occupancy and of defects such as steps or pits.

**S1Z215** **Prediction of Magnetic Flux Density Distribution in Soft Magnetic Materials Using 2D-FEM and Neural Network**

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Artificial Neural Network (ANN) and Finite Element Method (FEM) have recently been used for the prediction of magnetic performance in electromagnetic devices made from soft magnetic materials. In these materials, flux density distribution must be known for power loss calculation, material selection and core design. In this research, the flux density distribution in toroidal wound cores built from 0.27 mm thick M4 material at different magnetising frequency has been obtained using FEM and compared the nominal flux density values obtained in the previous measurements, having the same geometry. The obtained FEM results and experimental data used as a training data to a self organising feature map neural network for the prediction of flux density distribution. The network has been trained by Kohonen and back propagation algorithm. When the network was tested by untrained sample data, the linear correlation coefficient was found to be 98%.

## S1Z216

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Molecular dynamics has been used to simulate systems of mesoscopic size. We have implemented the bond order potential based on the tight binding scheme, using analytical expressions of the local density of states up to four moments and allowing for environmental screening of the underlying tight binding bond integrals. The obtained potential derives the interatomic forces from the local electronic density of states and thus proves superior to the Tersoff potential, often used for semiconductors, as it accounts naturally for the $\pi$-bonds and successfully reproduces the structural trends of silicon in various atomic arrangements. This is especially important for the simulation of wafer bonding with rotationally mis-aligned wafers as the atomic coordination at the interface may deviate substantially. We have applied this potential to model the atomic processes at bonding interfaces of silicon and diamond wafers.

## S1Z217 Self-interaction correction in the multiple-scattering representation: Application to the Ce $\alpha - \gamma$ phase transition

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We present a KKR implementation of the self-interaction-corrected LSD formalism and apply it to the well-known $\alpha$-$\gamma$ transition of Ce. Finite temperature calculations, including the disordered local moment (DLM) treatment for the paramagnetic $\gamma$-phase and the SIC-CPA are employed to calculate the phase-diagram and in particular the critical point of the transition. It is discussed how the treatment of the intermediate valence of the $\alpha$-phase influences the picture, and a strategy for treating this intermediate valence is outlined.

## S1Z218 INFLUENCE OF DEFECTS ON THE ELECTRONIC PROPERTIES OF CADMIUM TUNGSTATE SCINTILLATION CRYSTALS

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As well known and at the same time perspective scintillation crystal, cadmium tungstate CdWO4 is the subject of intensive experimental and theoretical investigations. Despite a plenty of works, the origin of luminescence in cadmium tungstate is still not clear enough. The electronic structures of several molecular clusters of cadmium tungstate crystals are ab-initio calculated by Hartree-Fock method using GAMESS program [1]. The oxygen vacancies and the molybdenum impurities are modeled in clusters. The electronic states of luminescence centers of cadmium tungstate are evaluated. Possible schemes of the luminescence processes in cadmium tungstate are proposed.

[1] Schmidt M.W., Baldridge K.K., Boatz J.A., et al.
J.Comput.Chem. - 1993. - v. 14. - p. 1347-1363.

S1Z219 **A novel method for calculating crystal field excitations in solids**

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A novel method for calculating crystal field excitations in solids is derived. Details in the implementation of the method in an all electron, first principles, full-potential, linear muffin-tin orbitals method are given. Numerical data for the crystal field exciations of elemental Pr, Pr-pnictides and PuO2 are compared to experiment, and the agreement is found to be good. The developed theory is also contrasted to traditional methods for calculating crystal field excitation, and a comparison is made. Finally, we describe future developments in theory of crystal field excitations.

S1Z220 **All-electron and pseudopotential calculations for PZT**

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Perovskites of the $PbZr_{(1-x)}Ti_xO_3$ (PZT) type are the most important ferroelectric materials. The main aim of the current study was the comparison of the results obtained using a pseudopotential code (ABINIT) with those of precise all-electron calculations. The latter were obtained using the FPLO (full-potential local-orbital) calculation scheme. Both schemes are based on density functional theory in local-density approximation. The structural and electronic ground state properties of PZT were studied for $x = 0.00$, 0.25, 0.50, 0.75, and 1.00. Several types of the atomic pseudopotentials were tested. We found that the Teter extended norm-conserving pseudopotential gives most reliable results for all compositions, the lattice constant being slightly underestimated compared with that given by FPLO. The pseudopotential code was used for the optimization of the crystal structure. The resulting ground state crystal structures are in good agreement with experiment and other theoretical calculations.

S1Z221 **Structure of Plain and Stepped BaTiO$_3$ Surfaces**

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In the framework of miniaturization of semiconductor devices ferroelectric compounds in the perovskite structure attract much interest. For example one of our aims is to deliver a density-functional based understanding of an organic field effect transistor on a ferroelectric template like $BaTiO_3$. Because of the low computational costs the density-functional based tight binding (DFTB) method allows one to study complex and large structures. Therefore in a first step we chose this technique to perform calculations on the relaxation of plain and stepped surfaces with a slab model geometry. Trends for the interplanar spacings and the local coordination at the step edge are discussed for vicinal (10n) surfaces.
In a further step by analyzing the distribution of the charge density and the polarizability we investigated possible positions for adsorbing organic molecules representing the switching element of the FET.

S1Z222 **Exchange interactions in spin glass alloys**

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We calculate the pair exchange interactions between magnetic atoms in fcc spin glass alloys (AuFe and CuMn) from first principles using the magnetic force theorem. The magnetic frustrations and the asymptotic behavior of the exchange interactions are strongly concentration dependent: with increasing concentration of magnetic atoms the interactions become shorter-ranged, their damping (with respect to the interatomic distances) has exponential character and the system becomes less frustrated since the antiferromagnetic interactions are damped more strongly than the ferromagnetic ones. It thus seems that the short-ranged theories of spin glasses are more appropriate for metallic systems.The results show that the standard RKKY theory is valid only in the low concentration limit. The calculated parameters can be used for realistic simulations of spin glasses.

S1Z223 **AB INITIO STUDY OF C14 Fe-Mo LAVES COMPOUNDS**

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We performed ab initio calculations of electronic structure of C14 Laves phases in the Fe-Mo system using the pseudopotential VASP code. The exchange-correlation energy was evaluated within the GGA approximation. The total energies of formation of Laves phase structure with various occupations of the sublattices ($A_2A$, $A_2B$, $B_2A$, $B_2B$) were evaluated with respect to the standard element reference states (SER). The calculated energy of formation of $Fe_2Mo$ with respect to the SER states is slightly positive (2.43 mRy/atom). However, this compound is more stable than the weighted average of the Laves phases of pure constituents (by 26.3 mRy/atom). On the other hand, the $Mo_2Fe$ compound is unstable with respect to both the SER states and the weighted average of the Laves phases of pure constituents. This research was supported by the Grant Agency of the Czech Republic, Projects Nos. 106/03/P002 and 106/02/0877.

S1Z224 **High pressure diamond-like liquid carbon**

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We report density-functional based molecular dynamics simulations, that show that, with increasing pressure, liquid carbon undergoes a gradual transformation from a liquid with local three-fold coordination to a 'diamond-like' liquid. This unusual structural change is well reproduced by the empirical bond order potential with isotropic long range interactions LCBOP, supplemented by torsional terms. In contrast, state-of-the-art short-range bond-order potentials do not reproduce this diamond-like structure.

**S1Z225** **The influence of local coordination polyhedra on bonding properties in Al-TM(transition metal) alloys**

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Among the aluminum transition-metal alloys the approximants of quasicrystals deserve particular interest, due to their anomalous electronic transport properties. Recently, covalent bonds in $\alpha$-AlMnSi were experimentally observed[1] which sheds light on the importance of the local atomic environment and hybridization in such systems. These findings support the idea that distinct transition-metal networks may exist in these approximants and that they have a crucial influence on the establishment of pseudogaps and high resistivities. By means of a tight-binding LCAO-method[2] and ab initio calculations the occurence of covalent bonds, the corresponding pseudogap in the density of states and the spectral resistivity are analysed with respect to the local coordination polyhedra in these networks. [1] Kirihara K. et al. (2003), Phys. Rev.,**B68**,014205 / [2] Slater, J.C. and Koster, G.F. (1954), Phys. Rev., **94**,1498

**S1Z226** **Conductance, polarisation and strength of Drude singularity in quantum junctions**

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We revisit the expression for the conductance of quantum junctions as obtained from the linear response theory [1]. For the unidirectional external electric field we derive a formula for conductance in terms of irreducible polarisation of the interacting system. The latter shows that the conductance represents the strength of the Drude singularity in the conductivity. We demonstrate that one can obtain the conductance of quantum junctions from calculations on finite systems without the need of special boundary conditions. Our expression is directly applicable to modern *ab-initio* methods (DFT, GW,...).
[1] P. Bokes and R. W. Godby, cond-mat0403204, accepted in Phys. Rev. B (2004).

**S1Z227** **Ground properties of transition metal disordered alloys: a KKR-CPA study**

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In this contribution we report on the results of the ground property calculations for several transition metal disordered alloys $M_{1-x}M'_x$ (M, M' = Fe, Ti, Ni, Cr, V, Nb, Mo, Ta, Pd). The calculations have been carried out using the charge and spin self-consistent KKR-CPA-LDA (Korringa-Kohn-Rostoker coherent-potential and local density approximation) method. The equilibrium lattice constants, bulk modulus, as well as the alloy formation energies were determined. Based on the concentration dependencies of the calculated formation energies the solid solution phase diagrams were reconstructed. We find them in fair agreement with available experimental data. For several of the present alloys the influence of the hydrogen insertion on the structural stability was investigated.

S1Z228 **Relaxation of interface defects: elastic boundary conditions and bond order potentials in empirical molecular dynamics simulations**

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Molecular dynamics simulations have been performed to investigate the relaxation of defects created during adhesion of semiconductor interfaces. The atomic processes at interfaces determine the behaviour of extended defects at a microscopic level, thus influencing the macroscopic properties of materials. To consider sufficiently large model sizes and relaxation times suitably fitted empirical potentials of the Tersoff type or analytically derived 4th momentum tight binding bond order potentials are applied and compared with respect to different structural details. In addition, the systems are coupled elastically to the bulk continuum surroundings rather than using periodic boundary conditions. The coupling is performed through the elastic multi-pole expansions for the displacement fields in the continuum region derived from an extended Lagrangian, with the expansion coefficients being treated as dynamic variables along with the positions of atoms in the atomic region. The simulations allow to predict the bonding processes and forces of perfect or disturbed surfaces against steps, facets, reconstructions, adsorbates, etc. The main focus, however, is on the networks of screw dislocations and arrays of 60 dislocations resulting from a twisted orientation and bonding over steps, respectively.

# Plenary Session 8:30 – 10:00 Hall A

P2A1 **Bond-order potentials : bridging the electronic to atomistic modeling hierarchies**

David Pettifor[1]

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The simulation of materials properties and processing often involves linking across the modeling spectrum from the quantum mechanical electronic level through the atomistic and microstructural to the classical continuum level. This talk focuses on bridging the gap between the electronic and atomistic modeling hierarchies by deriving interatomic bond-order potentials through coarse graining the electronic structure via atom-centred moments and bond-centred interference paths. The resultant interatomic bond-order potentials are discussed in relation to modeling the mechanical proprties of transition metals and intermetallics and to simulating the growth of semiconductor films.

P2A2 **Nanomechanical Systems**

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Nanoelectromechanical systems (NEMS) offer unprecedented opportunities for sensitive chemical, biological, and physical measurements with functionality down to the single-molecule limit. In vacuo, NEMS provide high force and mass sensitivity, ultimately below the attonewton and single-Dalton level respectively. In fluidic media, even though the high quality factors attainable in vacuum become precipitously damped, the small device size and high compliance yield response at the piconewton level – the force required to break individual hydrogen bonds within a macromolecule. Ultimately NEMS will provide access to the regime where mesoscopic mechanics becomes dominated by quantum, rather than thermal, fluctuations, and measurement sensitivity approaches, or even exceeds, the standard quantum limit.

# Focused Sessions 10:30 – 12:00

*New frontiers in Bose-Einstein Condensation* **Room B**

F2B1 **The physics of rapidly rotating Bose-Einstein condensates**

Gordon Baym[1]
*1) University of Illinois*

The energetically favored state of a rapidly rotating Bose condensed gas is, as observed, a triangular lattice of singly quantized vortices. What is the fate of the vortices when the rotation rate $\Omega$ is sufficiently rapid that the vortex cores would touch? Does a rotating Bose gas have a transition analogous to that observed in Type II superconductors at the upper critical magnetic field, $H_{c2}$? This talk will describe possible fates of the vortex lattice at large rotation in both harmonic and anharmonic traps. The vortex core sizes in a symmetric lattice approach a limiting fraction of the intervortex spacing, precluding a transition associated with core overlap. While a system in a harmonic trap at $\Omega$ very close to the transverse trapping frequency becomes quasi two-dimensional and can ultimately enter a quantum Hall-like state, a system confined in a trap steeper than harmonic enters a variety of new states, including a multiply-quantized giant vortex.

F2B2 **Spatial period-doubling in Bose-Einstein condensates in an optical lattice**

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*2) NORDITA, Blegdamsvej 17, DK-2100 Copenhagen, Denmark*

We demonstrate that there exist stationary states of Bose-Einstein condensates in an optical lattice that do not satisfy the usual Bloch periodicity condition. Using the discrete model appropriate to the tight-binding limit we determine energy bands for period-doubled states in a one-dimensional lattice. In a complementary approach we calculate the band structure from the Gross-Pitaevskii equation, considering both states of the usual Bloch form and states which have of the Bloch form for a period equal twice that of the optical lattice. We show that the onset of dynamical instability of states of the usual Bloch form coincides with the occurrence of period-doubled states with the same energy. The period-doubled states are shown to be related to periodic trains of solitons.

F2B3 **Tonks gas of ultracold atoms in an optical lattice**

Belén Paredes[1], Artur Widera[2], Valentin Murg[1], Olaf Mandel[2], Simon Fölling[2], Ignacio Cirac[1], Gora V. Shlyapnikov[4], Theodor W. Hänsch[3], Immanuel Bloch[2]
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*2) Institut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz, Germany.*
*3) Sektion Physik, Ludwig-Maximilians-Universität, Schellingstrasse 4/III, D-80799 Munich, Germany.*
*4) Laboratoire Physique Thèorique et Modèles Statistique, Université Paris Sud, Bâtiment 100, 91405 Orsay Cedex, France.*

Strongly correlated quantum systems are among the most challenging and intriguing systems in physics. Here the Tonks-Girardeau gas proposed about 40 years ago, is especially remarkable. In such a gas, bosonic particles are confined to one dimension, and they are prevented to be at the same position in space due to the strong repulsive interactions between them. This mimics Pauli's exclusion principle, resulting in pronounced fermionic properties of the bosonic particles. Interestingly however, these fermionized bosons do not exhibit either completely ideal bosonic or fermionic quantum behaviour, which is for example reflected in their characteristic momentum distribution. Here we report on the preparation of a Tonks-Girardeau gas in an optical lattice. We measure the momentum distribution and compare it with our theoretical prediction based on a fermionization approach, observing a remarkable agreement.

*Ferromagnetic semiconductor materials and spintronic devices*　　　**Room C**

F2C1　　**Magneto-optic effects and magnetization dynamics in metallic ferromagnetic semiconductors**

Jairo Sinova[1]
*1) Texas A&M University*

Metallic diluted magnetic semiconductors materials offer a much wider spectrum of magneto-transport, magneto-optics and collective effects than conventional itinerant electron ferromagnets, mostly due to the greater tunnability of the Mn moments ordered state through growth conditions, doping, gates, and light. Here we study the properties of metallic (III,Mn)V semiconductors based on the itinerant hole-fluid model. We will discuss the different results and predictions of the model and its agreement to experiments such as magnetization dynamics, magneto-optic effects, and magneto-trasport effects. Beyond its success we emphasize the need to further explore the new predictions which it offers to sharpen our understanding of these fascinating materials.

F2C3　　**Spintronic nanostructures**

Laurens W. Molenkamp[1]
*1) Physikalisches Institut(EP3), Würzburg University*

Advances in our theoretical unsderstanding of spininjection phenomena, as well as in materials related technolgy development, have allowed us to start exploring spintronic effects in semiconductor nanosctructures.

As a first example of such devices, I will present a resonant tunneling diode fabricated from a paramagnetic II-VI semiconductor, that can be operated as a voltage controlled spin-switch. A further example is the observation of a very large spin valve effect occurring at sub-10 nm sized constrictions in a ferromagnetic semiconductor GaMnAs. This type of device allows the experimentalist to cope with the very short spin scattering length in this material. Finally, I will address the origins of a spin valve-like behavior we have observed in tunnel structures containg a GaMnAs layer. The observations imply that TMR-like behavior in magnetic tunnel structures signals does not necessarily provide evidence for spin-polarized tunneling.

*Plutonium-based Superconductivity* **Room D**

### F2D1 Magnetic and superconducting behavior in PuRhGa5 and related compounds

F. Wastin[1], E. Colineau[1], J. Rebizant[1], P. Javorsky[2], P. Boulet[1], J.C. Griveau[1], G.H Lander[1]
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The superconductivity recently observed in the intermetallic compounds PuCoGa5 [1] and PuRhGa5 [2] is a new direct evidence of plutonium anomalous electronic behavior. The high critical parameters (Tc of 18.5K and 9K respectively), displayed by these compounds together with strong analogies with the heavy-fermion d-waves CeMIn5 family of superconductors, make of the PuMGa5 a new fascinating class of materials with still a lot of open questions. In this paper we will review the magnetic and superconducting behaviors of PuRhGa5 and related compounds.

[1] Sarrao et al., Nature 420, 297 (2002)
[2] Wastin et al., J. Phys.: Condens. Matter 15, S2279 (2003).

### F2D2 Tuning unconventional superconductivity in $CeMIn_5$ and $PuMGa_5$

J.L. Sarrao[1]
*1) Los Alamos National Laboratory*

Superconductivity has recently been discovered in $PuCoGa_5$ at $T_c$=18.5 K, nearly an order of magnitude larger than in the isostructural heavy fermion superconductor $CeCoIn_5$ ($T_c = 2.3$ K). The superconducting properties of $PuCoGa_5$ including the power law dependence of the specific heat, the temperature-pressure phase diagram, and, in particular, the linear variation of the c/a ratio of the tetragonal lattice parameters with $T_c$, bear a striking resemblance to the unconventional superconducting properties of $CeCoIn_5$. The remarkable similarities between the $CeMIn_5$ (M=Co, Rh, Ir) and $PuMGa_5$ (M=Co, Rh) families of superconductors, taken together with the occurrence of superconductivity in the presence of strong magnetic correlations, suggests a common mechanism of superconductivity, possibly magnetically mediated, that is quite effectively tuned structurally and/or by the increased bandwidth of Pu relative to Ce. The similarity between the $PuMGa_5$ and $CeMIn_5$ superconductors and its implications will be discussed.

### F2D3 Electronic structure of the Pu-based superconductors $PuCoGa_5$ and $PuRhGa_5$

Peter M. Oppeneer[1], Ingo Opahle[2], Saad Elgazzar[2]
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The electronic structure of the novel Pu-based medium-high-$T_c$ superconductors $PuCoGa_5$ and $PuRhGa_5$ is investigated on the basis of *ab initio* density functional calculations. We also performed calculations for related non-superconducting actinide 115 compounds. The lattice parameters are well reproduced when we assume delocalized $5f$ states. The possibility of a partial $5f$ localization is discussed. Our total-energy calculations predict antiferromagnetic order to be favorable for all three Pu-115 materials, which is, however, observed experimentally for $PuIrGa_5$ only. Possible origins of the unexpected superconductivity are discussed. Our investigation particularly reinforces the analogy to the heavy-fermion superconductors $CeCoIn_5$ and $CeIrIn_5$, however, with a stronger coupling strength due to a much stronger $5f$ hybridization.

*Soft condensed matter at large* **Room E**

### F2E1 **Fluctuations of model membranes: complementarity of neutron and x-ray studies**

Giovanna Fragneto[1], Edith Bellet-Amalric[2], Alan Braslau[3], Thierry Charitat[4], Jean Daillant[3], Francois Graner[5], Barry Stidder[5]

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*2) DRFMC/SP2M/SGX, CEA Grenoble (F)*
*3) SPEC CEA, Gif-Sur-Yvette (F)*
*4) Institut Charles Sadron, Strasbourg (F)*
*5) Universite Joseph Fourier, St-Martin-d'Heres (F)*

Biophysical studies of membrane-membrane and membrane-protein interactions require well controlled model systems. A new method for obtaining single phospholipid bilayers floating in excess water near an adsorbed bilayer at the solid-liquid interface, has been developed recently. The structure and fluctuation spectrum of the floating bilayers were determined by combining neutron specular reflectivity and synchrotron radiation off-specular reflectivity measurements. A minimum of the bilayer bending modulus was found for phosphocholines around the main phase transition. Besides the bending modulus determination, off-specular synchrotron data have allowed the determination of the bilayer tension both in the gel and fluid lipid phases. This was the first time that the technique was applied to single lipid bilayers at the solid/liquid interface. Neutron specular reflectometry was also used to study floating bilayers containing varying amounts of cholesterol. It was found that while amounts of cholesterol of about 10 mol

### F2E2 **CRYSTALLINE THIN FILM ARCHITECTURES AT THE AIR-LIQUID INTERFACE**

Leslie Leiserowitz[1]
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The use of grazing incidence X-ray diffraction (GIXD) using synchrotron radiation for the characterization of thin crystalline films composed of amphiphilic molecules at the air-aqueous solution interface, shall be discussed. This opening section will include a brief description of the GIXD experimental setup at Hasylab, Hamburg. Various topics based on crystalline architectures at the air-solution interface will be covered. This will include the use of amphiphilic monolayers for induced nucleation of organic and inorganic three-dimensional (3D) crystals at the air-solution interface and the spontaneous separation of left and right-handed molecules to form 2D crystals of opposite handedness. Finally we shall cast some light on pathological crystallization of cholesterol, which precipitates in gallstones and atherosclerotic plaques, via the use of GIXD for trapping the cholesterol nucleation process.

F2F1  **Growth Dynamics of Pentacene Thin Films**

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The growth of pentacene thin films is of major importance for the development of organic thin film transistor displays. In particular, the pentacene transistor mobility depends significantly on the crystalline quality of the organic material in the channel and on the contacts of the device. Here we present an in-situ study of pentacene MBE growth on Si and Au surfaces. On clean Si, up to 50 $\mu$ m large pentacene crystallites are formed that grow in the thin-film phase. The dendritic shape of these islands will be analyzed and simulated in the framework of diffusion limited aggregation (DLA). The growth of pentacene layers can be modified, and to some degree controlled, by pre-adsorption of simple organic monolayers. Au films as substrates for pentacene can be prepared in-situ at elevated temperatures. At low coverages, Au forms a (5x2) reconstruction on the Si(111) substrate, and pentacene is again observed to grow in the thin film phase. At coverages beyond 3/4 ML of Au a (?3x?3) reconstruction is formed that causes the orientation of the pentacene film to rotate by almost $90^o$. The same result is found for pentacene on thick polycrystalline Au films. Again, the adsorption of organic self-assembled monolayers (SAMs) prior to deposition of pentacene can restore the growth direction of pentacene to a crystal orientation as seen on Si and on $SiO_2$.

F2F2  **PTCDA on Ag - a model system for organic epitaxy**

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We present the results of a systematic growth study of 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) on Ag(111). The organic thin films have been deposited by molecular beam epitaxy and studied by in situ x-ray diffraction and atomic force microscopy. A transition between layer-by-layer growth and islanding has been observed which smears out as a function of temperature. This transition is accompanied by morphological and structural changes. Many aspects of structure and growth can be related to similar observations on very different material systems such as metals and semiconductors.

F2F3    **The Role of Triplet Excitons in Organic Electronic Devices**

Stephen Forrest[1]

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It has been found that triplet excitons have numerous uses in organic electronic devices, especially in organic light emitting devices and photovoltaic cells. For example, metallorganic complexes employing a heavy metal provides strong spin-orbit coupling that allows for efficient intersystem crossing in the ligand, resulting in efficient luminescence from the molecular triplet state. This has been used in demonstrating OLEDs with ∼100% internal quantum efficiency in the green, and 60-80% internal efficiency in the red and deep blue. Indeed, more recently, triplet excimers have also proven to be efficient means for generating white light emission. We have exploited the properties of triplets in both OLEDs and PV cells, and in both cases these devices have improved properties well beyond those achieved in singlet-only devices. The efficient harvesting of triplet states by metallorganic compounds in electrophosphorescent OLEDs has provided us with an unprecedented opportunity to investigate their dynamics, and this will be the primary topic of the talk. I will also describe the properties of devices employing triplets. Furthermore, I discuss measurements of the singlet-triplet exciton formation ratio in both polymers and small molecular weight organic materials. In both cases there is significant direct as well as inferential data to suggest a purely statistical formation ratio of 25% singlets to 75% triplets by electrical injection. Prospects for the study and use of these excited state species will also be considered.

*Physics of the cascade lasers* **Room G**

### F2G1 Antimonide quantum cascade lasers

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Quantum cascade lasers (QCLs), widely used now to produce coherent radiation from the mid- to far-infrared spectral region, are based mainly on two material systems: GaInAs/AlInAs on InP substrates and GaAs/GaAlAs on GaAs substrates. The antimonide materials with the lattice parameter near 6.1 $\mathring{A}$, such as GaSb, AlSb and InAs, are very promising for the development of QCLs because of the large $\Gamma$ point conduction band offset of 2.0 eV for the InAs/AlSb systems. We will first discuss on the physical parameters that influence the performance of QC lasers in the different material systems, then present a study of InAs/AlSb QCLs carried out within the framework of a joint program of the University of Montpellier and Thales R&T.

### F2G2 Modelling of quantum cascade lasers

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Quantum Cascade Lasers have become an important source for infrared spectroscopy within the last decade. While standard simulations for these structures are based on semiclassical rate equations, a quantum transport description is needed to study coherent effects, Here the theory of nonequilibrium Green functions allows the performance of transport and gain simulations [1]. The results predict the possibility of gain down to 1.5 THz [2]. Taking into account the electron-electron interaction we find that the depolarisation shift gives a blue shift for the absorption at lower frequencies but hardly affects the gain spectrum itself [3].
[1] Lee and Wacker, PRB **66**, 245314 (2002). [2] Lee and Wacker, APL **83**, 2506 (2003). [3] Pereira, Lee, and Wacker, PRB, in press, cond-mat/0404015.

*From femto towards attosecond time scale in solids* **Room H**

F2H1 **Extreme nonlinear optics with few-cycle pulses in semiconductors**

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If a semiconductor is excited by very intense few-cycle optical pulses, unusual things can happen: Frequency doubling can occur in the presence of inversion symmetry, signals may depend on the phase between the carrier wave and the envelope of an optical pulse and large light-induced gaps can occur. The talk gives an introduction starting from a very basic level and reviews some of our corresponding recent experiments.

F2H2 **Time resolved attosecond spectroscopy: looking into atoms**

GA Reider[1], M Drescher[2], L Manojlovic[1], R Kienberger[1], E Goulielmakis[1], M Uiberacker[1], V Iakovlev[1], F Krausz[1]

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An overview is given of the state of art in optical attosecond pulse generation and measurements. The interaction of intense laser pulses with rare gas atoms results in the emission of XUV pulses of sub-femtosecond duration - the current minimum pulse duration is about 200 attoseconds. To yield single, isolated attosecond pulses, the driving laser pulses need to be controlled precisely in terms of their intensity envelope and absolute phase. Combined with a time resolving correlation technique that relies on the interaction of electrons with a strong laser feld it is possible to measure attosecond electron dynamics from systems excited by these ultrashort XUV pulses. Photo-electron emission as well as Auger-electron emission are well suited processes for this novel time resolved spectroscopy. The extension of current gas phase experiments to solid surfaces is discussed.

F2H3 **Ultrafast X-ray diffraction**

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Until a few years ago the only means of studying ultrafast phenomena was optical pump-probe spectroscopy using femtosecond light pulses. This situation is changing rapidly, because the generation of femtosecond pulses in the X-ray regime has recently become possible. Ultrashort X-ray pulses now enable femtosecond time-resolution to be extended to X-rays and X-ray spectroscopy. Ultrafast X-ray diffraction combines atomic scale spatial and temporal resolution enabling extremely rapid changes in the atomic configuration to be directly observed.

*Physics of nanomaterials* **Hall J**

F2J1 **Growth and structural properties of low-dimensional nanostructures**

J. Stangl[1], R.T. Lechner[1], Z. Zhong[1], F. Schaeffler[1], G. Springholz[1], T.U. Schuelli[2], V. Holy[3], G. Bauer[1]
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A survey on the growth of group IV (Ge/Si) and of IV-VI compound nanostructures grown by molecular beam epitaxy on (001) and (111) oriented substrates will be presented. Short range lateral ordering of Ge or PbSe Stranski-Krastanow islands is induced by elastic interactions, which also leads to island ordering along the growth direction for proper spacer layer thicknesses. However, the huge elastic anisotropy present in IV-VI compounds leads even to a trigonal or hexagonal three-dimensional ordering of PbSe islands embedded in PbEuTe if grown along the [111]- direction. Long range ordering of islands can be induced by a proper combination of prepatterning of the substrate and self-assembled growth. For Ge islands on Si (001) it can be shown that a two-dimensional periodic arrangement of pits in the Si substrate determines the nucleation sites of Ge islands, which grow at the bottom of the pits. By growing an island multilayer on such a substrate, a three- dimensional island crystal is formed, as evidenced by x-ray diffraction data. Finally it will be shown that a template consisting of hexagonally ordered PbSe islands can be used to induce the self-organized growth of magnetic EuSe islands.

F2J2 **Nanosecond dynamics of magnetic films and nanostructures**

R. C. Woodward[1], K. J. Kennewell[1], D. C. Crew[1], R. L. Stamps[1]
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The rapid advance in magnetic data storage has been a driving force for fundamental research in magnetism in two simultaneous directions. The first is the drive towards the behaviour of nanoscale magnetic entities. As we reduce the size of an entity into the nanometer regime there is an increasing importance of interface effects. The second area of fundamental interest is in the nanosecond time regime. In this regime we move from a time frame where properties are determined by thermal activation over energy barriers, to times where the angular momentum and the associated precessional behaviour of the magnetic spins dominate. We will examine the behaviour of materials that have at least one dimension restricted to the nanometer regime as we approach times scales of the order of nanoseconds. We will also investigate the changes in properties observed in some simple materials as we modify the interface and how, as the interface effects become predominant, the behaviour of the systems becomes increasingly more complex.

F2J3 **Investigation of Defects in Ultra Fine Grained Metals by Positron Annihilation Spectroscopy**

Jakub Cizek[1], Ivan Prochazka[1], Bohumil Smola[1], Ivana Stulikova[1], Radomir Kuzel[1], Zdenek Matej[1], Viktoria Cherkaska[1], Miroslav Cieslar[1], Rinat K. Islamgaliev[2], Olya Kulyasova[2]
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*2) Institute of Physics of Advanced Materials, Ufa State Aviation Technical University, Russia*

Microstructure and thermal stability of bulk ultra fine grained (UFG) metals (grain size around 100 nm) prepared using severe plastic deformation (SPD) were investigated. Microstructure studies were performed by positron annihilation spectroscopy (PAS) combined with TEM and XRD. Dislocations represent a dominant type of defects. Vacancy clusters (so called microvoids ) represent another kind of defects introduced by SPD. Recovery of UFG structure with temperature is realized by the abnormal grain growth, followed by recrystallization, i.e. grain growth in the whole volume. Temperature intervals of these processes and corresponding activation energies were investigated.

# Mini-Colloquia 14:00 – 16:00

*Turbulence in coherent quantum systems and connections to general hydrodynamics*
**Room B**

### M2B1 Numerical simulation on quantum turbulence

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This paper describes the recent theoretical and numerical research on quantum turbulence and the dynamics of quantized vortices. A quantized vortex is a topological defect characteristic of quantum fluid, being much different from a vortex in a classical viscous fluid. Quantum turbulent state consists of a disordered tangle of quantized vortices. Although our understanding of these topics has made significant gains since the early studies, the recent interest has shifted to the nature of superfluid turbulence, apart from the old works chiefly of counterflow. After briefly stating the properties of quantized vortices and the current motivations on this field, we discuss the recent activity, with emphasis on the contribution made by our group. First, we show that superfluid turbulence consisting of a vortex tangle has an energy spectrum consistent with the Kolmogorov law. Second, we discuss the vortex states that appear in a rotating channel with counterflow; the competition of rotation and counterflow makes a new state of a polarized vortex tangle.

### M2B2 Creation and decay of quantum turbulence in He II

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Except at the very lowest velocities, the flow properties of He II are dominated by the production and decay of quantized vortex lines. It is now known that the creation of vortex line *ab initio* is a relatively rare process. Quantum turbulence (QT) – a dense tangle of quantized vortex lines – usually arises through processes that expand remanent vortex lines pre-existing in the liquid. The present status of QT in He II is reviewed briefly. Surprisingly, recent work has shown that QT can often behave in a manner very similar to classical turbulence. This could conceivably be associated with the presence of viscous normal fluid component in the range of temperatures $T > 1$K where the experiments were performed. Partly to help resolve this question, new flow experiments in the $T \to 0$ limit, where the normal fluid component is effectively absent, are in progress.

### M2B3 Turbulence in rotating superfluid ³He-B

A. Finne[1], V. Eltsov[1], J. Kopu[1], M. Krusius[1], L. Skrbek[1], E. Thuneberg[1], G. Volovik[1]
*1) Low Temperature Laboratory, Helsinki University of Technology, Finland*

The first measurements on superfluid turbulence in ³He-B have been conducted in the last few years. New understanding is expected, since ³He-B displays a different perspective on turbulence, which so far is extensively known only from ⁴He-II. The major differences are a large viscosity of the normal component, mutual friction damping of vortex motion with wide range of variation as function of temperature, and the possibility to use different measuring techniques which answer new questions. The main new result is a sudden transition from regular vortex number conserving dynamics to turbulence, with decreasing damping. This change is driven by the Kelvin-wave instability of a single vortex line when it starts to move with the applied superflow at sufficiently low damping. Of great interest is the configuration in which vortex loops injected into vortex-free superflow expand in a long column under uniform rotation, and the zero temperature limit behavior when the normal component (the hydrodynamic reference frame) and dissipation vanish.

*Physics of f-electron materials II. (PCFES 7)*                    **Room C**

## M2C1  The magnetic response of an antiferromagnetic superconductor, $UPd_2Al_3$

Elizabeth Blackburn[1], Arno Hiess[2], Nick Bernhoeft[3], Gerry H. Lander[1]
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*2) Institut Laue-Langevin, BP 156x, F-38042, Grenoble, France*
*3) DRFMC, CEA-Grenoble, F-38054, Grenoble, France*

Information on the interplay between superconductivity and magnetism is key to our understanding of a large variety of materials, such as heavy-fermion superconductors. An excellent example is the heavy-fermion compound $UPd_2Al_3$ which orders antiferromagnetically at $T_N = 14$ K and becomes superconducting at $T_c = 2$ K. We used cold-neutron three axis spectroscopy to measure the magnetic response of this compound in high magnetic fields. We present a review of the experimental results obtained in magnetic fields up to $B = 15$ T in the normal state. The magnetic response shows intriguing temperature and field dependent behaviour that can be linked to the superconductivity, reflecting the characteristic properties of the electronic system.

## M2C2  Polarisation of Spin Waves in $UO_2$

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*2) European Commission, JRCITU, D-76126 Karlsruhe, Germany*
*3) Institut Laue Langevin, BP 156 X, F-38042 Grenoble, France*

Spherical neutron-polarimetry has been applied to study the nature of magnetic fluctuations propagating along the symmetric directions $\Delta$, $\Sigma$ and $\Gamma$ in the ordered phase of $UO_2$. For $\vec{q} \parallel [00\zeta]$, the acoustic spin-wave branch is linearly polarized over a large fraction of the zone, whereas the two branches at higher energy are isotropic. For $\vec{q} \parallel [\zeta\zeta0]$, the acoustic mode is anisotropic from the magnetic zone center up to the magnetic zone boundary, where it becomes suddenly isotropic. The optic branches are, on the contrary, isotropic near the magnetic and nuclear zone centers, but anisotropic around the magnetic zone boundary. A varying anisotropy has been observed also along the $[\zeta\zeta\zeta]$ propagation direction. The experiments open a perspective on a more detailed understanding of the exchange interactions in many different systems.

## M2C3  Stability of AF structure in UNiAl in magnetic fields

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The hexagonal UNiAl orders antiferromagnetically (AF) below $T_N$=19.3K. In zero field below $T_N$, the AF reflections are indexable using the propagation vector $q_{old}$=(0.1 0.1 0.5). When a magnetic field is applied along the c axis, UNiAl undergoes a sharp metamagnetic transition at $B_c$=11.35T (4.2K) towards the ferromagnetic phase. Some time ago magnetic history dependent phenomena were revealed in UNiAl, which concern all the bulk properties. Neutron diffraction studies revealed that below 7 K in fields higher than 8-9T the original AF structure diappears and a new AF structure characterized by $q_{new}$=(0.173 0 0.5) appears. The higher the field (but smaller than $B_c$) the faster the development of the new AF structure is observed. After releasing the field the old AF structure reappears. The process is seemingly thermal activated.

M2C4 **Ligand NMR Studies of Neptunium Compounds**

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A recently initiated program of neptunium compound synthesis at our center has allowed us to carry out studies of NMR and susceptibility behavior in $NpO_2$ and $Np_2MGa_5$, where M is typically a 3d metal ion. NMR data on $^{17}O$ in $NpO_2$ show a line structure below the ordering temperature $T_C = 25.5K$ which reveals two inequivalent oxygen sites. This is consistent with the triple-q octupolar-quadrupolar ground state proposed on the basis of X-ray scattering studies by Paixão, *et al.* $T_1$ data show a general absence of divergent behavior near $T_0$, but also display an anomalous field dependence over a wide range of temperatures. For the 115 series, $Np_2FeGa_5$ appears to be a semi-metal with antiferromagnetic ordering at $T \sim 120K$. Single crystal $^{69,71}Ga$ NMR shift and relaxation data from the paramagnetic state of this and other compounds will be discussed.

*Quantum criticality in heavy-fermion metals and ruthenates* **Room D**

M2D1 **Metamagnetism and quantum fluctuations in the ruthenate $Sr_3Ru_2O_7$**

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Quantum criticality may provide a unified framework for understanding many facets of strongly correlated electron behaviour in solids. In addition, entirely novel behaviour is often seen in the close vicinity of quantum critical points.

In this talk we will discuss the bilayer ruthenate metal $Sr_3Ru_2O_7$ where we will present evidence for the existence of a magnetic-field-tuned quantum-critical point and discuss its nature. Furthermore, we will show unusual properties in its vicinity that may indicate the presence of a novel form of quantum order.

M2D2 **Hall effect at a heavy-fermion quantum critical point**

S. Paschen[1]
*1) Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*

Several experimental observations indicate that a new type of quantum critical point (QCP), different from the Hertz/Millis spin density wave (SDW) type, may exist in certain heavy-fermion metals. The magnetic field-induced QCP of $YbRh_2Si_2$ might be of such an unconventional type. Here we use Hall measurements to address the question of whether, in $YbRh_2Si_2$, the Fermi surface transformation at the QCP develops gradually as expected if the magnetism is of SDW type, or suddenly as expected if the heavy electrons are abruptly localized by magnetism.

In collaboration with: T. Lühmann, S. Wirth, P. Gegenwart, O. Trovarelli, C. Geibel, F. Steglich, P. Coleman, and Q. Si.

M2D3 **Magnetic fluctuations close to an antiferromagnetic quantum critical point as observed in Ce(Cu,Au)6 and CeNi2Ge2**

A. Schroeder[1]
*1) Kent State University, Kent OH*

Neutron scattering spectra of the heavy fermion compounds Ce(Cu,Au)6 and CeNi2Ge2 will be presented to characterize the magnetic correlations and dynamics close to an antiferromagnetic quantum critical point. While the magnetic response in Ce(Cu.Au)6 reveals quantum critical fluctuations which can be consistently described in a simple, although unconventional picture, the situation in CeNi2Ge2 is more complex, both defying the "ideal" conventional scenario expected for a three dimensional antiferromagnetic quantum critical point.

**M2E1** **Magnetocaloric properties of Fe(Mn) based intermetallics for room temperature magnetic refrigeration**

O Tegus[1], B Fuquan[1], L Zhang[1], W Dagula[1], E Bruck[1], F.R. de Boer [1], K.H.J. Buschow[1]
*1) Van der Waals-Zeeman Instituut, Universiteit van Amsterdam, Valckenierstraat 65,1018 XE Amsterdam, The Netherlands*

During the last few years we have studied the magnetic and magnetocaloric properties of a variety of intermetallic compounds based on Fe and/or Mn in order to find materials that lend themselves for magnetic refrigeration near room temperature. The prerequisite for the latter application is a Curie temperature near room temperature associated with a sufficiently large magnetocaloric effect. Our efforts have concentrated mainly on compounds of the hexagonal Fe2P structure type, because the latter offers the possibility of numerous substitutions into the metal site as well as into the nonmetal site. Particularly promising results were obtained for compounds in which there is a field-induced first-order magnetic phase transition slightly above the Curie temperature.

**M2E2** **Application of the itinerant-electron metamagnetic transition in $La(Fe_xSi_{1-x})_{13}$ compounds to high-performance magnetic refrigerants by hydrogen absorption**

A Fujita[1], K Fukamichi[1]
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We have first demonstrated that the field-induced first-order magnetic transition from the paramagnetic to the ferromagnetic state, namely, the itinerant-electron metamagnetic (IEM) transition takes place above the Curie temperature $T_C \sim 200$ K in $La(Fe_xSi_{1-x})_{13}$ compounds. Large magnetocaloric effects (MCEs) due to the IEM transition are induced by low magnetic fields around $T_C$. To obtain the large MCEs around room temperature, $T_C$ is increased by hydrogenation with keeping the IEM transition. Large values of the isothermal entropy change $\Delta S_m \sim$ -28 J / kg K and the adiabatic temperature change $\Delta T_{ad} \sim 7$ K are obtained at 300 K in 2 T for $La(Fe_{0.90}Si_{0.10})_{13}H_{1.1}$. Therefore, $La(Fe_xSi_{1-x})_{13}H_y$ can be utilized as high-performance magnetic refrigerants in a wide range of temperature covering room temperature in relatively low magnetic fields.

**M2E3** **Comparison of MnAs and GdGeSi intermetallics under pressure in terms of the colossal magnetocaloric effect**

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The compounds MnAs and Gd5Ge2Si2 are similar in terms of their physical properties. Their Curie temperatures (Tc) are close to 300 K and the first order magnetic transition is coupled to a structural one, showing a great volume change, revealing a high magnetoelastic coupling. They are important materials for magnetic refrigeration due to their giant magnetocaloric effect. Under hydrostatic pressure, however, they present dissimilar behaviors. For MnAs Tc decreases with pressure, the thermal hysteresys increases and the magnetocaloric effect becomes colossal. For Gd5Ge2Si2 Tc increases, the hysteresys remains almost constant and the magnetocaloric effect decreases. In this work we discuss these behaviors experimentally and in the light of a phenomenological model.

M2E4 **The Magnetocaloric Effect in Intermetallic Compounds and their Role in Magnetic Refrigeration**

Karl A. Gschneidner, Jr.[1]
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The magnetocaloric effect (MCE) is the response of a magnetic solid to the application or removal of a magnetic field. When subjected to a magnetic field the magnetic moments are aligned and the magnetic entropy is lower. Under adiabatic conditions the total entropy remains constant, and thus the sample heats up. When the field is removed the magnetic entropy is increased and the temperature is lowered. The MCE is strongly dependent upon the magnetic ordering process. It is substantial for second order magnetic transitions, and it is generally the largest for first order magnetic transitions. A number of the giant MCE materials have been studied over the past seven years. These include: the $Gd_5(Si_xGe_{1-x})_4$ based alloys, the rare earth manganites, the lanthanum-iron-silicon [$La(Fe,Si)_{13}$] alloys and manganese based alloys. Various concerns regarding the utilization of magnetic refrigerants in magnetic cooling will be discussed.

M2E5 **Interplay of structure and magnetism in $R_5(Si_xGe_{1-x})_4$**

L. Morellon[1], C. Magen[1], P. A. Algarabel[1], C. Ritter[2], Z. Arnold[3], M. R. Ibarra[1]
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*3) Institute of Physics AS CR, Na Slovance 2, 182 21 Prague 8, Czech Republic*

$R_5(Si_xGe_{1-x})_4$ is a unique family of intermetallics where an interesting and exotic behavior has been recently discovered. Their exceptional magnetoresponsive properties such as the giant magnetocaloric effect, strong magnetoelasticity, and giant magnetoresistance have triggered an active research, more than 100 scientific papers being published since 1997. This phenomenology has been associated with the intrinsically layered crystallographic structure combined with a magnetic-martensitic-like first-order phase transformation. In this contribution we will review the outstanding properties of these materials and our recent findings on the effect of hydrostatic pressure on the phase transitions in selected compounds of this family, especially in the parent $Gd_5Ge_4$ alloy.

M2E6 **Strong magnetocaloric effect in transition-metal compounds**

H. Yamada[1]
*1) Faculty of Science, Shinshu University, Matsumoto 390-8621, Japan*

Recently, transition-metal compounds $MnFe(As,Sb)$ and $La(Fe,Si)_{13}$, which exhibit either temperature- or field-induced first-order magnetic phase transition, have attracted much attention, because they are promising materials for the magnetic refrigeration. In this paper, we discuss such temperature- and field-induced transitions on the theory of itinerant-electron metamagnetism, and discuss an isothermal magnetic entropy change. The effect of spin fluctuations is taken into account by phenomenological Ginzburg-Landau theory. It is generally shown that a strong magnetocaloric effect in itinerant-electron metamagnets is expected when the coefficient of the fourth order of the magnetization in the Landau energy expansion with respect to the magnetization is negative and large. The Landau coefficient can be estimated by the analysis of the observed magnetization curve, and also by ab initio band calculations in the fixed-spin-moment method. $CoS_2$ and $Fe(Si,Ge)$ are shown to be good candidates for magnetic refrigerators.

*Physics in high magnetic fields* **Room F**

M2F1 **Nuclear Magnetic Resonance in High Pulsed Magnetic Fields**

J. Haase[1], B. Buechner[1], M. Kozlov[1], D. Eckert[1], H. Eschrig[1], K.H. Mueller[1], H. Siegel[1]
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Nuclear Magnetic Resonance (NMR), a powerful research tool, is typically performed in high, stable magnetic fields with great homogeneity for improving sensitivity and resolution. High magnetic fields also serve as an external tuning parameter for the study of modern materials electronic properties that NMR can detect. Since the highest magnetic fields can only be achieved with pulsed magnets one may ask whether it is possible and useful to perform NMR in such magnets. First NMR spectra at up to 60 T, the new world record for high field NMR, show the feasibility. Challenges from the time dependence of the field, its homogeneity and short rise time will be addressed and solutions will be presented. It will be shown that NMR in pulsed high field magnets is a promising research tool not only for the highest fields.

M2F2 **Localized, Itinerant, and Superfluid Spin Triplons in Quantum Magnets**

Marcelo Jaime[1]
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Quantum magnets contain spin-1/2 dimers in their lattices of $Cu^{2+}$ ions. The ground state is a product of singlet spin-dimers, separated by an energy gap of a few meV from the spin triplet excited state. If a magnetic field is applied, the triplet state splits via the Zeeman effect. Once the applied magnetic field exceeds a critical value, a gas of $S = 1$ triplet excitations or *triplons* is stabilized. At low temperatures this bosonic gas can either crystallize or liquefy. The liquid state is a strong candidate to become a magnetic superfluid. I will discuss specific heat and magnetization results at magnetic fields higher that the critical fields in the Shastry-Sutherland compound $SrCu_2(BO_3)_2$ and Han purple $BaCuSi_2O_6$. The former shows clear evidence for crystallization of triplons, while the later seems to undergo Bose-Einstein condensation of a spin liquid.

M2F3 **Suppression of interlayer coupling in semiconductor bi-layers in high magnetic fields**

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Semiconductor bilayers are two sheets of two dimensional electron gases (2DEG) separated by a thin barrier, which exhibit new degrees of freedom due to the interlayer coupling. In the experiment quantum oscillations in the resistance are measured as a function of magnetic field (up to 33T) and low temperatures at different tilt angles with respect to the plane of the layers. It is found that the addition of an in-plane field effectively tunes the interlayer coupling, suppressing it altogether in very high parallel fields. Consequently all interlayer phenomena disappear with tilt angle, and most spectacularly the sample switches from metallic to insulating in the quantum limit by changing the angle only a few degrees.

M2F4 **Nexus Between Quantum Criticality and Phase Formation: The Case of URh2Si2**

J. A. Mydosh[1]
*1) Max Planck Institute for Chemical Physics of Solids, Dresden, Germany*
*2) Also at Kamerlingh Onnes Laboratory, Leiden University, The Netherlands*

Quantum criticality is becoming increasingly recognized as a controlling factor in the creation of novel phases, e.g. unconventional superconductivity. However, direct proof for a causal link between the quantum fluctuations and the phase formation remains a formidable experimental challenge. URu2Si2 is an example of a strongly correlated electron system where signatures of quantum criticality appear at very strong magnetic fields indicating the existence of a quantum critical point (QCP) hidden beneath a complex region of interconnecting phases. Using a variety of thermodynamic and transport measurements we map out the field/temperature phase diagram and establish the QCP at 37 T. We then show how Rh doping simplifies the phase diagram eliminating all but one of the phases while preserving the robust QCP.

M2F5 **Bose-Einstein condensation of the triplet states in the magnetic insulator $TlCuCl_3$**

Ch. Rüegg[1], A. Furrer[1], K. Krämer[2], H.U. Güdel[2], P. Vorderwisch[3], K. Habicht[3]
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*2) Department of Chemistry and Biochemistry, Universität Bern, Switzerland*
*3) BENSC, Hahn-Meitner-Institut Berlin, Germany*

Inelastic neutron scattering (INS) has been used to investigate the unconventional field-induced ordered phase of dimer quantum spin liquids. The magnetic insulators $XCuCl_3$ with X=K, Tl represent a family of such compounds. The two $Cu^{2+}$ ions forming the dimer in a 3D network are antiferromagnetically (AF) coupled resulting in a singlet ground-state. At a critical external magnetic field $H_c$ the singlet-triplet gap is closed, offering a unique opportunity to explore a field-induced quantum phase transition, which may be considered as the BEC of triplet magnon excitations. The INS spectra at $H > H_c$ show the coexistence of a novel mode, which has a linear dispersion around the field-induced AF Bragg point, with renormalized quadratic Zeeman modes of dimer origin.

*Multiscale modelling*                                                    **Room G**

M2G1    <u>**Novel aspects of the dislocation mechanisms in DC covalent crystals.**</u>

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Covalent crystals are ideal materials to study dislocation multiplication and mobility in the presence of a lattice friction. Such mechanisms are revisited in intrinsic Ge single crystals deformed between 700 and 1000K, using original transient tests (creep, stress relaxation and dip tests).
Before the upper yield point, intense dislocation multiplication is evidenced during the transients: i) after the transient the yield point is lower ii) transient curves are very different from those of metallic crystals. They are analysed in terms of multiplication laws proposed successively for metals, covalent crystals and one derived from 3D computer simulations in Si. None of them satisfactorily describes the transient curves, very likely because they ignore strain localization.
At larger strains the thermal and the internal stress are separated using dip tests. The former suggests a single deformation mechanism at all temperatures. The latter corresponds to long range elastic interactions of dislocations. Surprisingly, it depends on temperature and strain-rate, as the microstructure does. Activation energy values, static and dynamic TEM data suggest that the dislocations overcome a lattice friction combined with point obstacles such as debris or impurities.

M2G2    <u>**Bridging the length scales by hybrid molecular dynamics**</u>

Michael Moseler[1], Matous Mrovec[2], Christian Elssser[1], Peter Gumbsch[2]
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The simulation of localized energetic disturbances in solids has to bridge several length scales. Atoms far from equilibrium (for instance in the impact region of a particle-solid collision, in dislocation cores or in crack tips) should be described with quantum precision e.g. by tight binding or computational more expensive methods. The partially disordered zone surrounding the quantum region can be treated with semi-empirical many body potential (for instance, bond order potentials). Finally, the two atomistic zones are embedded into a continuum with macroscopic stress or strain boundary conditions. Special attention has to be paid to the coupling of the different media requiring a) a coherent elastic behaviour of the whole system and b) a strong reduction of high frequency elastic wave reflection at zone boundaries. The performance of hybrid molecular dynamics is demonstrated for the energetic collision of a carbon cluster with a diamond surface.

M2G3    <u>**From an ideal crystal to a microstructure: Multiscale modeling of bcc transition metals**</u>

Matous Mrovec[1], Christian Elsässer[2], Michael Moseler[2], Peter Gumbsch[1]
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Isolated extended defects such as dislocations or grain boundaries can be treated nowadays with high accuracy by electronic-structure methods (e.g. DFT). These methods are unfortunately still not capable to proceed to more complex cases such as interaction of extended defects with each other, or polycrystals subjected to externally applied stresses. At this level of complexity one has to cross the bridge between the electronic-structure modeling and the atomistic modeling, where the electronic degrees of freedom are coarse-grained into many-body interatomic potentials. We focus on specific problems and solutions for bcc transition metals which are known to be more difficult to handle theoretically than close-packed metals. We will discuss various descriptions of interatomic interactions, their reliability and possible coalescence into multiscale modeling schemes.

M2G4  **Mixing and separation in binary alloys of transition metals**

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Formation of microstructure is influenced by the tendencies towards formation of ordered structures on one side, and separation of phases with prevailing concentration of one element on the other side. Description of interatomic forces respecting metallic character of bonding using many-body potentials is analysed first for various fcc elements and then for their binary alloys. It is demonstrated to which extent this description can reproduce different elastic and alloying behaviour. Such analysis is helpful for applications of these potentials in models of complex structures of extended defects such as dislocation and interfaces and in assessment of their properties.

M2G5  **Towards a Multiscale Modelling of Adhesive Joints:
Extending Atomistic Simulations to the Interphase**

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The mechanical properties of adhesive joints are determined by the direct interaction zone between substrate and adhesive. It is shown that computational predictions of the properties of the interphase necessitate a multiscale approach. As a first step towards a multiscale treatment, we examine the surface chemistry of silica and alumina and predict atomistic structures of model surfaces by density functional tight binding (DFTB). Possible reactions of the organic components present in commerical adhesives with the surfaces are examined. In order to extend the applicability of these atomistic simulations to larger scales, a novel QM/MM approach utilizing DFTB is introduced. Structures obtained by QM/MM for the organic components are compared to ab initio results.

M2G6  **Theoretical strength and high-strain elasticity of intermetallic compounds
from first principles**

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Under a high-strain deformation, material may transform to some other structure or fracture. The instabilities correspond to the theoretical strength of the material. We give an account of applications of quantum-mechanical electronic structure calculations to the problem of high-strain elasticity and theoretical tensile strength in intermetallic compounds $Ni_3Al$, $MoSi_2$ and $WSi_2$ that are very promising as high-temperature structural materials. The anisotropy of elastic properties at high strains is explained in terms of higher-symmetry structures present or absent along the corresponding deformation paths. The role of relaxation of internal structure parameter in transition metal disilicides is discussed and changes in bonding conditions during the tensile test are analyzed.

*Boron-based III-V compound semiconductors* **Room H**

M2H1 **Photoluminescence and structural investigation of BGaAs/GaAs epilayers**

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We report on the growth conditions of the alloy BGaAs, followed by optical and structural investigation of BGaAs/GaAs epilayers. Epilayers were obtained by Metal Organic Chemical Vapor Deposition (MOCVD), with boron composition up to x=0.075. Photoluminescence spectroscopy (PL) as a function of the excitation density and the sample temperature (10-300 K) has been done. We have seen how the optical properties varied versus the sample temperature and excitation density. The experimental results indicate that the band gap of the BGaAs shifts to low energy side compared to the GaAs one. An enhanced exciton-localization like mode for the BGaAs epilayer is observed.

M2H2 **Preparations and semiconducting properties of boron phosphide and boron antimonide**

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*1) Yokohama National University*
*2) Nihon University*

We have been studying boron compound semiconductor to develop new electric materials (1).The present paper reviews our studies on boron phosphide and boron antimonide films at the last decade. Firstly, the fundamental optical properties of BP wafers were studied using resonant soft X-ray emission and absorption spectra(2).The absorption edge and its low-energy tail on Si-doped B12P2 wafer were optically determined(3). An isotope substitution effect in BP single crystalline wafer was confirmed by the measurements of precise lattice parameters by Bond method and Raman spectra(4). Secondly, the electrical and thermal properties of boron phosphide wafers and films by ambient(5-9) and low pressure(10,11) CVD processes were examined. Recent our results on BP films on SOI and sapphire (R-) plane were explained. Z value for n- and p-type BP films on SOI substrates showed 10-4~10-3/K, and 10-5~10-4/K, respectively, at 700-1000K. That for p-BP on sapphire R-plane showed 10-5~10-4/K at 700-900K. Finally, we proposed newly designed BSb based on band(12) and quantum chemical calculations. A B12Sb2 films by molecular flow region PVD process displayed high mobility of ~100cm2/V.s and high Z value of ~10-4/K(14) which would make the film promising candidates for new functional device materials. References (1) Y.Kumashiro:J.Mater. Res.5.2933 (1990): Electric Refractory Materials p.557,Marcel Dekker Inc.New York (2000).(2) A.Agui et als.J.Phys.Soc.Jpn., 68 199(1999).(3) H.Werheit et als.J.Alloys & Comp. 233,121(1996).(4) Y.Kumashiro et als. J.Cryst. Growth 132,611(1993).(5) id. J.Solid State Chem.133 269(1997).(6) id. ibid.154 33(2000).(7) id. ibid.154 39(2000).(8) id. ibid.177 529(2004).(9) id. ibid.133 314(1997).(10) id. ibid.154 26(2000)(11) Y.Kumashiro: Landort-Brõuml;nstein, Semiconductors.Vol3/41A1$\beta$ p.122 Springer-Verlag, Berlin. (2002). (12) Y.Kumashiro et als. J.Solid State Chem. 177,533(2004) (13) id. J.Cryst. Growth 237-239,1531(2002)(14) id. J.Solid State Chem. 133,104(1997).

M2H3 **Epitaxial growth 3C-SiC on Si(100) substrate using a BP buffer layer**

Yoshihisa Abe[1], Jun Komiyama[1], Syunichi Suzuki[1], Hideo Nakanishi[1]
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3C-SiC is one of wide band gap materials, and is particularly attracted on its cubic structure, which is able to apply a lot of the mature Si technologies. It is well known that 3C-SiC grows usually on Si substrates. However, the high degree of lattice mismatch between 3C-SiC and Si has caused the generation of defects. We attempt to use cubic BP as buffer layer, in terms of the reduction of these interfacial defects between 3C-SiC and Si substrate. The BP was grown on Si(001) substrates by $B_2H_6$ and $PH_3$ at $950°C$. We adopted a thin SiC layer grown at temperatures lower than $900°C$ as a SiC growth template, because BP decomposes at temperatures higher than $900°C$. The SiC template layer was grown on BP/Si(001) by monomethylsilane($CH_3SiH_3$) about $800°C$. And SiC growth was carried out at $1150°C$ by $SiH_4$ and $C_3H_8$ on the template layer. The effect of the lattice relaxation using BP buffer layer for 3C-SiC growth on the Si substrate are clearly demonstrated by XRD measurements.

M2H4 **Structural investigation of hetero-interface of transparent (111)-BP layer and (111)-GaP substrate**

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*2) Electronics Materials Division, Electronics Sector, Showa Denko K.K.*

Crystallographic feature of BP layer grown on lattice-mismatched (111)-GaP substrate was evaluated by means of transmission electron microscopy (TEM). The BP layer grown by MOCVD using triethylboran and phophine sources was transparent. The BP layer grew epitaxially on the (111)-GaP with relation:(111)[110]-GaP//(111)[110]-BP. Presence of (111)-microtwins in the (111)-BP layer was also revealed. By high-resolution TEM observation, an irregular alignment of crystal planes of the BP was found at the interface with the GaP. Growth manner of the BP layer is discussed with relation to the formation of the microtwins and the irregular alignment of the crystal planes.

M2H5 **Direct-bandgap properties of hexagonal boron nitride**

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To achieve compact laser devices for use in deep UV region, many researchers are devoting considerable effort to finding materials with larger direct band gaps than that of GaN. In this paper, we show that hexagonal boron nitride (hBN) is a promising material for UV laser devices because of its direct band gap nature in UV region. A pure hBN single crystal, which proves it to be a direct bandgap material by showing a dominant cathodoluminescence peak at 215 nm, and a series of s-like exciton absorption bands around 215 nm, was obtained by employing a high-pressure and high-temperature method. Based on the absorption spectrum, the bandgap energy of 5.971 eV and the quasi-two dimensional exciton binding energy of 149 meV were finally obtained. In addition, UV lasing at 215 nm by accelerated electron excitation was demonstrated at room temperature as proved by the enhancement of the longitudinal mode and threshold behavior of the excitation current dependence of the emission intensity.

M2H6    <u>**Bonds and bands in boron compounds**</u>

A. ZAOUI[1]
*1) RWTH-Aachen, Germany*

Boron compounds (BN, BP, BAs and BSb) have attracted increasing research interest over the past few years, as wide-gap semiconductors. These materials are of great technological interest for high-temperature, electronic and optical applications. This is due to their unique physical properties such as low densities, extremely high thermal conductivities, wide band-gap and large resistivities. In addition to their interesting properties, these materials possess some peculiar characteristics that I will discuss and try to explain in this contribution. Among these peculiar characteristics is the inverse role between the cation and the anion in terms of charge transfer and the new phase transition. The latter aspect does not obey the Phillips diagram established for semiconductors compounds, which predicts a metallic structure as the first new transition phase for weakly ionic compounds such as BP, BAs and BSb. The main reasons for these fundamental differences between these compounds and other materials will be discussed.

*Quantum dots for quantum computing* **Hall J**

M2J1 <u>**All-Optical Detection of Electron Spin in a Single Quantum Dot**</u>

Atac Imamoglu[1], Mete Atature[1]
*1) ETH Zurich*

A single quantum dot with an excess conduction band electron is an ideal system to study quantum optical phenomena in semiconductors. In this talk, I will describe recent progress in our experimental work aimed at all optical electron-spin measurement. Further, I will highlight the direction of our efforts for observing electron spin flips in real time.

M2J2 <u>**Quantum computation using electrons trapped by surface acoustic waves**</u>

Crispin H. W Barnes[1]
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I will describe a set of ideas for implementing flying qubits, quantum gates, and quantum gate networks in a semiconductor heterostructure device. These ideas are based on an extension of the technology used for surface acoustic wave (SAW) based single-electron transport devices. These devices allow single electrons to be captured from a two-dimensional electron gas in the potential minima of a SAW. I show how this technology can be adapted to allow the capture of electrons in nearly pure spin states and how both single and two-qubit gates can be constructed using magnetic and nonmagnetic gate technology. I give designs for spin readout gates and discuss how combinations of gates can be connected to make a quantum processor. I will also discuss decoherence and other sources of error, and how they can be minimized for this type of quantum processor.

M2J3 <u>**Site- and Energy-Controlled Semiconductor Quantum Dots for Quantum Information Processing Applications**</u>

Eli Kapon[1]
*1) Laboratory of Physics of Nanostructures, Swiss Federal Institute of Technology Lausanne (EPFL), Switzerland*

Quantum information processing applications would greatly benefit from site-controlled semiconductor quantum dots (QDs) with well-defined excitonic states. We have developed (In)GaAs/(Al)GaAs QD systems using organometallic chemical vapor deposition on patterned GaAs substrates. The dots self-form at the centers of inverted pyramids made using lithography. Optical spectroscopy of single pyramidal QDs reveals reproducible neutral and charged excitonic states. Photon correlation spectroscopy is utilized to observe single- and cascade-photon emission from these structures. Record-low (4meV) inhomogeneous broadening is measured for ordered dot arrays. Adjustment of the QD ground and excited states using substrate pattern modification is demonstrated. The incorporation of such pyramidal QDs into active photonic crystals is also discussed.

# Poster Session 16:00 – 18:00

S2X1 **Magnetoelasticity of $R_2 T_{13.6} Si_{3.4}$ ($R$ = U, Lu; $T$ = Fe, Co)**

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Uranium and 3d metals do not form the binary intermetallic compounds with the 2-17 stoichiometry. Nevertheless, the $Th_2Ni_{17}$ hexagonal crystal structure can be stabilized by relatively small amount of Si. We have grown the single crystals of the $U_2 T_{13.6} Si_{3.4}$ ($T$ = Fe, Co) compounds and the corresponding analogues with Lu. The magnetoelasticity has been studied by the magnetization measurements under ambient and high pressure in fields applied along the main axes and by the x-ray diffraction thermal-expansion measurements. The results are discussed in assumption of a magnetic state of U in $U_2Fe_{13.6}Si_{3.4}$ and a non-magnetic one in $U_2Co_{13.6}Si_{3.4}$.

S2X2 **LDA+U calculation of the crystal field interaction in PrO$_2$**

Martin Diviš[1], Ján Rusz[1], Vladimír Nekvasil[2]

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*2) DMS, IOP, CAS, Cukrovarnická 10, 162 53 Prague 6, Czech Republic*

$PrO_2$ is an insulator with the band gap of 6 eV. The $4f^1$ ground state configuration of $Pr^{4+}$ in cubic symmetry sites is subjected to a strong crystal field (CF) interaction. The available inelastic neutron scattering data show that the ground state symmetry CF state $\Gamma_8$ and the excited $\Gamma_7$ symmetry state are separated by 130 meV. This energy separation is described by a single CF parameter $A_4^0 = -661 K$. The standard local density approximation (LDA) gives the gap value of 3.7 eV and the CF parameter $A_4^0 = -59 K$. The LDA+U based approach, where the Coulomb correlations inside the Pr-5d and O-2p states is described using the parameters U = 0.5 Ry and J = 0.1 Ry, results in the band gap value of 6 eV and $A_4^0 = -107 K$. These results indicate that while the LDA+U method gives better description of the electronic structure than LDA, it is too crude to describe the CF interaction in the rare earths insulators at the semi quantitative level.

S2X3 **EXPERIMENTAL STUDY OF MAGNETOCALORIC EFFECT IN DIPOLAR SPIN ICE Dy$_2$Ti$_2$O$_7$**

A. Vlček[1], M. Orendáč[1], A. Orendáčová[1], T. Fennel[2], S. T. Bramwell[2]

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*2) Department of Chemistry, University College London, 20 Gordon Street, London WC1H0AJ, UK*

The magnetocaloric effect of dipolar spin ice $Dy_2Ti_2O_7$ was experimentally investigated in the temperature range 0.28 K - 8 K and in the magnetic field up to 2 T. The field induced adiabatic temperature change above 1 K can be well described using the temperature and magnetic field dependence of the magnetic entropy as calculated from the magnetic specific heat data. Cooling during the adiabatic demagnetization below 1 K can be attributed to the change of the residual entropy caused by magnetic field. The results of the demagnetization at various sweeping rates suggest that $T_{min} \approx 0.25 K$ might represent the lowest temperature obtainable by the demagnetization of $Dy_2Ti_2O_7$.

S2X4 **Transport and Magnetic Properties of (Sr,A)RuO$_3$ (A = K, Na)**

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*2) Dep. Quimica e Bioquimica, CCMM, FCUL, 1749-016 Lisboa, Portugal*
*3) Dep. Fisica, CFMC-UL, FCUL, 1749-016 Lisboa, Portugal*

SrRuO$_3$ is generally considered as a ferromagnetic metal with T$_C \sim$160 K, the electrical behaviour pointing to a strongly correlated bad metal. Previous works concerning the Sr substitution by Ca or ions of different valence (as La) tried to clarify the interplay between electrical and magnetic properties and the lattice structural distortion. However, the overall behaviour is not yet well understood. In this work, electrical resistivity and magnetization measurements as a function of T and H were performed in (Sr,A)RuO$_3$ (A=K,Na). A decrease of T$_C$ and effective moment were observed with the increase of A content, more significantly in the case of Na, maintaining the overall ferromagnetic behaviour. Electrical resistivity measurements are consistent with these results exhibiting a marked transition from metallic to T$^2$-behaviour at the ordering temperature.

S2X5 **Origin of the negative volume magnetostriction of GdAl$_2$ compound**

Ilja Turek[1], Ján Rusz[2], Martin Diviš[2]
*1) Institute of Physics of Materials, Academy of Sciences of the Czech Republic, Brno*
*2) Department of Electronic Structures, Charles University, Prague, Czech Republic*

The contribution is focused on the GdAl$_2$ intermetallic compound with the cubic C15 Laves structure which exhibits a negative magnetostriction, in contrast to majority of metallic magnets. We present results of ab initio calculations which employ a disordered local moment (DLM) state as a model for a reference paramagnetic state. The electronic structure of the DLM state is treated in the coherent potential approximation. The calculated lattice parameters reproduce both the negative sign and the magnitude of experimentally observed magnetostriction. We explain the negative magnetostriction by a volume dependence of the indirect Gd-Gd exchange interactions. The latter are evaluated in the framework of a classical Heisenberg Hamiltonian with exchange parameters derived from the selfconsistent electronic structure of the ferromagnetic state. The calculated Curie temperature agrees with experiment as well.

S2X6 **Intra and inter layer magnetic coupling of V in Cu0.5(VOAsO4)**

F. C Tsao[1], T. -N Li[2], P. J Hwung[1], M. K Chung[1], C. C Yang[1], K. -H Lii[2], W. -H Li[1]
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*2) Department of Chemistry, National Central University, Chung-Li, 32054, Taiwan*

Magnetism in layered structures has currently attracted considerable attentions. The compound Cu0.5(VOAsO4), where V atoms are surrounded by O atoms to form 2D V-O networks which are connected by As-O tetrahedral and Cu atoms. We has successfully fabricated Cu0.5(VOAsO4) by employing hydrothermal synthesis method. AC Magnetic susceptibility was measured to study the basic magnetic behaviors of the compound. Three transitions of magnetic in nature were observed at 63, 54, and 45 K. The V moments in the 2D layers order ferromagnetically below 63K. Interlayer couplings become evident below 54 K, reflecting the appearance of domain enhancement effect. The transition at 45 K can be due to the reorientation of the V moments. Details will be discussed.

S2X7 **Spin Canted Polaritons in Ultra-Thin Antiferromagnet Films**

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We consider the propagation of spin canted magnetic polaritons in thin antiferromagnets $XF_2$ (X=Mn,Fe) unsupported ultra-thin films. We use the Voigt configuration where the direction of propagation is perpendicular to the magnetic moments and to the applied external magnetic field. We obtain analytical equations for the dispersion relations, both in the magnetostatic regime and retarded region, and we show that they reduce to previous expressions for simpler cases. Numerical results for the polariton spectra are then obtained, which show, besides the expected non-reciprocal effects, a rich profile with surface and guided polariton modes. For the experimental point of view, the spectra can be probed by far-infrared resonance (FIR) spectroscopy in either grating or Fourier-transform form.

S2X8 **X-RAY PHOTOELECTRON SPECTROSCOPY AND MAGNETISM OF THE $Al_4GdNi$ AND $Al_6GdNi_3$ COMPOUNDS**

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The paper tackles the X-ray photoelectron spectroscopy (XPS), the magnetization and the magnetic susceptibility of the compounds $Al_6GdNi_3$ and $Al_6GdNi_3$. In these compounds, the Ni 3d band is completely full. It is filled because of the kind of coordination of the Ni atoms, which brings about strong hybridization 3d. The Ni atoms do not carry a magnetic moment. In these compounds the magnetic order at lower temperatures is anti-ferromagnetic and it is based on the RKKY indirect coupling between the localized 4f spins of Gd ions. The complete filling of the Ni 3d band revealed by the density of the states at the Fermi level, the absence of the magnetic moments. The magnetic moment in excess in the case of the Gd ions is due to the contribution of the 5d electrons polarized by the local exchange interaction 4f-5d.

S2X9 **Searching for magnetism in palladium in face-centered and body-centered cubic crystal structure**

T. Káňa[1], D. Legut[2], M. Šob[3]
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*2) Inst. Phys. Materials, Acad. Sci. Czech Rep., Brno, Czech Rep.*
*3) Inst. Theor. Phys. Chem., Fac. Sci., Masaryk Univ., Brno, Czech Rep.*

An ab initio study of mechanical and magnetic properties of palladium with both fcc and bcc structure is presented. For both structures, total energies, magnetic moments and bulk moduli are calculated. We use the linearized augmented plane wave method implemented in the Wien2k code. The calculations are performed within both local spin density approximation (LSDA) and generalized gradient approximation (GGA). Results of the calculations show that palladium, crystallizing either in fcc or bcc structure, should be non-magnetic. The calculated results are compared with available experimental data.

## S2X10 **XMCD study of double perovskites (Sr,Ba,Ca)2FeReO6**

M. Sikora[1], D. Zajac[1], C.J. Oates[1], M. Borowiec[1], D. Rybicki[1], Cz. Kapusta[1], D. Serrate[2], J.M. De Teresa[2], M.R. Ibarra[2]
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*2) Instituto de Ciencia de Materiales de Aragn, Universidad de Zaragoza-CSIC, Spain*

Results of X-ray Magnetic Circular Dichroism (X-MCD) measurements of the A2FeReO6 double perovskites (A = Ca, Ba and Sr) at L2 and L3 edges of rhenium are reported. For all the compounds studied a strong negative (weak positive) X-MCD signal was observed at the L2 (L3) edge, which proves existence of a magnetic moment of 1 Bohr magneton at the Re site, antiparallel to Fe moments. Application of sum rules reveals a considerable orbital contribution to the Re moment, except for the dominant spin contribution. This provides an experimental proof for the model of magnetic interaction in the compounds, that involves overlapping spin down Fe(3d), O(2p) Re(5d) electron bands, which leads to half metallicity and magnetoresistive behaviour.

## S2X11 **Magnetocaloric effect in a pyrochlore magnets $Gd_2Ti_2O_7$**

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*2) Department of Physics, University of Warwick, Coventry UK*
*3) DMS/SPSMS/DRFMC CEA Grenoble, France*

The effect of an adiabatic demagnetization was experimentally studied in a frustrated pyrochlore magnet $Gd_2Ti_2O_7$. Decreasing the magnetic field from 12 T we observed a strong cooling of the sample in the field range 6-12 T corresponding to the crossover from saturated to a spin-liquid phase. The observed phenomenon indicates that the considerable part of the magnetic entropy associated with the macroscopic number of local soft modes survives below the Curie-Weiss temperature and acquire a gap at fields above the crossover. The results of classical Monte-Carlo simulations are in good agreement with the experiment. The cooling limit of the sample $T_{min} = 0.45$ K is determined by freezing out the residual entropy at the sequence of ordering transitions. The cooling power of the process is experimentally estimated.

## S2X12 **MAGNETIC PROPERTIES OF $Cu(NH_3)_2Ag(CN)_4$ - A QUASI 2D HEISENBERG ANTIFERROMAGNET**

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The experimental results of the susceptibility, specific heat, magnetization and electron - spin resonance of $Cu(NH_3)_2Ag(CN)_4$ are reported. Although the magnetic Cu(II) ions are arranged in a regular 2d square lattice, thermodynamic quantities significantly deviate from the behaviour expected for the corresponding 2d Heisenberg system. The deviation can be attributed to the entanglement of neihgbouring layers. The sudden increase of specific heat data observed below 300 mK suggests the onset of long-range order at lower temperatures.The mechanisms leading to the long-range order in the studied 2d system are discussed.

S2X14 **Nuclear Magnetism of PrPb$_3$ in the Antiferro-quadrupolar Ordered state.**

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*2) Low Temperature Physics Lab., RIKEN, Wako-shi, 351-0198, Japan*
*3) Faculty of Engineering, Kyusyu Institute of Technology, Kitakyusyu 804-8550, Japan*

The crystalline electric field (CEF) ground state of the intermetallic compound PrPb$_3$ is a non-magnetic $\Gamma_3$ doublet and the AntiFerro-Quadrupolar Ordering (AFQO) occurs at T$_Q$ = 0.4 K. We measured the static magnetization of PrPb$_3$ in the magnetic fields 0.94 and 6.21 mT down to 200 $\mu$K. In the AFQO state, the hyperfine-enhanced nuclear magnetic susceptibility increased below 40 mK followed by the Curie Weiss law, and showed a peak at 5 mK. The enhancement factor obtained from the Curie constant was 1+K = 30. The peak height at 5 mK was only $10^{-3}$ of the expected saturated magnetization. These results suggest that the hyperfine-enhanced nuclear magnetic moments of Pr order antiferromagnetically below 5 mK.

S2X15 **COERCIVITY PROPERTIES OF Gd/Si/Co MULTILAYERS WITH FERRIMAGNETIC ORDERING**

Yu.A. Shakhayeva[1], D.N. Merenkov[1], A.B. Chizhik[1], S.L. Gnatchenko[1], M. Baran[2], R. Szymczak[2], V.O. Vaskovskiy[3], A.V. Svalov[3]
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*2) Institute of Physics, Poland*
*3) Ural State University, Russia*

Coercive properties of ferrimagnetic multilayers [Gd75$\AA$/Si/Co30$\AA$] with thicknesses of silicon equal 2, 3, 5 $\AA$ have been investigated in the temperature range from 20 to 300 K. The coercive field H$_C$ is increased nearby of compensation point, where spontaneous magnetization M$_S$ is minimal. The temperature dependencies of coercivity are well described by ratio H$_C$=$\alpha$/M$_S$-NM$_S$, where N - demagnetizing factor. The dependencies H$_C$/M$_S$ from 1/M$_S{}^2$ are fitting by linear curve. $\alpha$ is remain constant in whole temperature range, and increased only at transition through a point of compensation. Thus, the changes of coercivity were related with changes of spontaneous magnetization.

S2X16 **Dependence of magnetic properties from thickness and content of material in ultrathin films.**

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The magnetic properties of ultrathin films with range of thickness from 0.3ML up to 15ML for FeNi allows deposited on a surface of copper (100), in particular, spin reorientation transition (SRT) in-plane and out-of-plane observed by means of methodic magnetooptical Kerr effect (MOKE), demonstrated the dependence of these transitions from percent quantity of iron in allows and defined by thickness (dc) viewed before. At these measurements a control of quality of films and a thickness by means of LEED, RhEED, Auger- spectroscopy were carried out. Deposition of allows went from two separated sources. The percent quantity of iron from 7% up to 25% in ultrathin films of FeNi allows shows the absence any kind of transitions for a thickness of some monolayers. We wonder to draw Your attention on this branch of iron concentrations and small $\Delta$ around curves near its, where present SRT for the consideration of effects and following use in nanoelectronics, element of magnetic recording.

S2X17 **A One-Dimensional Magnetic System; Terbium Borosilicide**

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Magnetism of various higher boride compounds is discussed. $AB_6$ systems have attracted interest ever since high temperature ferromagnetism was reported. However, we have previously carefully investigated the phenomena and were able to show the first strong proofs that they are non-intrinsic [1,2]. More boron-rich compounds such as $REB_{66}$ are well known, but the main interest has tended to be of structural or mechanical nature. However, recently interesting magnetic behavior was discovered in $B_{12}$ icosahedra-containing dilute f-electron compounds. For example, the 3D long range order of $GdB_{18}Si_5$, and 2D spin glass behavior of a series of higher borides like $HoB_{22}C_2N$ [3]. Results obtained for neutron diffraction and doping effects on $TbB_{44}Si_2$ are presented. It is indicated that this is a 1D system with extremely short range interaction. [1,2]T. Mori, S. Otani, SSC 123 (2002) 287, JPSJ 71 (2002) 1789. [3]e.g. T. Mori, H. Mamiya, PRB 68 214422 (2003).

S2X18 **Hydrogen-induced variations of U7Sn magnetism**

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Among uranium compounds crystallizing with the ZrNiAl structure type, only UNiAl has been known to absorb hydrogen. We report UCoSn and URuSn to absorb $\geq$ 0.7 H at. per formula unit under pressure 120 bar and $T$ = 923 K. No change in the structurte type was observed and the volume expansion is 3.2% for UCoSn and 1.2% for URuSn. The tendencies of magnetic properties differ for both compounds. While UCoSn exhibits a typical behaviour expected for intermetallics of uranium upon hydrogenation ($T_C$ increases from 82 K to 102.5 K, the spontaneous magnetic moment increases from 0.64 $\mu_B$/U to 0.70 $\mu_B$/U), the influence of hydrogen absorbtion on URuSn is opposite ($T_C$ decreases from 54 K to 51 K, its magnetic moment gets reduced - 0.48 $\mu_B$/U in $URuSnH_{0.7}$ comparing to 0.53 $\mu_B$/U in URuSn).

S2X19 **Magnetic properties of REPt$_3$Si**

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Motivated by the recent discovery of the co-existence of superconductivity ($T_c$ = 0.75 K) and antiferromagnetism ($T_N$ = 2.2 K) in non-centrosymmetric CePt$_3$Si, we investigate the crystal structure and magnetism of rare-earth (RE)-Pt$_3$Si compounds. Single phase compounds REPt$_3$Si have been obtained with RE= La to Gd, Dy, Tm and Y, where La- to GdPt$_3$Si are isostructural (simple tetragonal, P4mm), while Y-, Dy- and TmPt$_3$Si exhibit a significantly lower symmetry. The investigation of the magnetic properties by means of magnetic susceptibility, specific heat and magnetoresistivity measurements reveal antiferromagnetic order with $T_N$ = 3 K, 8 K, and 15 K for Nd-, Sm-, and GdPt$_3$Si, respectively, while the results obtained from PrPt3Si indicate a non-magnetic singlet ground state.

S2X20　**Precipitation of Magnetic Oxide in $_x$Fe$_2$O$_3$ (1-x) [MO 2B$_2$0$_3$] Glasses; The Effect of Magnetic Field during Precipitation**

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In oxide glasses some of the constituent oxides can be precipitated in the crystalline form by heat treatment at a suitable temperature. This is one of the well-known techniques for producing glass-ceramics; the suitable heat treatment temperature is indicated by Differential Thermal Analysis (DTA) curves of the glasses. In the case of glasses containing magnetic oxides, it is, therefore, interesting to study how the presence of the magnetic field affects the precipitation process of crystalline phase out of the amorphous matrix. In this paper we report the effect of the field on the crystallization behaviour of Fe$_2$O$_3$ in Pb, Sr and Ba Borate glasses containing varying concentration of Fe$_2$O$_3$. The aim of our study was to investigate whether the application of magnetic field of 0.8 T during the heat treatment at two temperatures indicated by DTA increased or decreased the amount of precipitated phase. The DTA curves of these glasses showed two peaks, one corresponding to magnetic phase Fe$_2$O$_3$ and another a nonmagnetic borate complex of alkaline earth oxide (PbO, BaO, SrO). The changes in the amount of Fe$_2$O$_3$ and the crystalline phase of borate complex were estimated from the x-ray diffraction patterns and the magnetization curves of the samples. Our results indicate that, in general, when the processing temperature is near the crystallization temperature of the magnetic oxide, the magnetic field aids the crystallization of the magnetic phase. However, when the heat treatment temperature is near the crystallization temperature of the nonmagnetic phase, application of the magnetic field diminishes the amount of the precipitated magnetic phase. A tentative explanation of this phenomenon is provided. We also observed that increasing the amount of magnetic oxide in the glasses led to a wider separation between the crystallization temperatures of the magnetic and the nonmagnetic phase. Our findings may have application in the manufacturing process of magnetic glass ceramics. We are continuing our study on simpler binary glasses where it is hoped that only the magnetic phase is separated.

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S2X21　**High pressure effect on ferromagnetic ordering in layered copper octacyanotungstate**

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Recently, new molecule-based magnets created on the [W$^V$(CN)$_8$]$^{3-}$ or [Mo$^V$(CN)$_8$]$^{3-}$ precursors, were synthesized and structurally characterized. The temperature dependencies of AC-susceptibility measured under pressure revealed a pronounced linear decrease of the Curie temperature with a pressure coefficient d$T_c$/dp = - 7.2 K/GPa. The identical value of d$T_c$/dp has been derived from M(T) dependencies and Arrots plots measured under different pressures. Almost negligible effect of pressure on magnetization M$_s$ points out to a localized character of magnetic moments in the studied octacyanotungstate.

## S2X22    **Magnetocaloric effect on TbCu$_2$ single crystal**

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Here we present the results of the detailed study of the magnetocaloric effect on the TbCu$_2$ single crystal in the temperature range $2 - 60$ K and in magnetic fields up to 3 T parallel to the crystallographic $a-$axis. The orthorhombic intermetallic compound TbCu$_2$ orders antiferromagnetically below the Néel temperature $T_N = 54$ K [1] yielding a colinear magnetic structure with the Tb magnetic moment parallel to the $a-$axis. In magnetic fields $B \approx 2$ T applied along this axis the structure undergoes a metamagnetic transition into the field-induced ferromagnetic phase which is accompanied by an abrupt change of the magnetic entropy. This change of entropy is compensated by the adiabatic change of the temperature of the crystal, i.e. causes the magnetocaloric effect (MCE). The detailed study of the magnetization enables us to evaluate the (MCE) using the well-known thermodynamic Maxwell relation.

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## S2X23    **The Magnetocaloric Effect in Intermetallic Compounds and their Role in Magnetic Refrigeration**

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The magnetocaloric effect (MCE) is the response of a magnetic solid to the application or removal of a magnetic field. When subjected to a magnetic field the magnetic moments are aligned and the magnetic entropy is lower. Under adiabatic conditions the total entropy remains constant, and thus the sample heats up. When the field is removed the magnetic entropy is increased and the temperature is lowered. The MCE is strongly dependent upon the magnetic ordering process. It is substantial for second order magnetic transitions, and it is generally the largest for first order magnetic transitions. A number of the giant MCE materials have been studied over the past seven years. These include: the Gd$_5$(Si$_x$Ge$_{1-x}$)$_4$ based alloys, the rare earth manganites, the lanthanum-iron-silicon [La(Fe,Si)$_{13}$] alloys and manganese based alloys. Various concerns regarding the utilization of magnetic refrigerants in magnetic cooling will be discussed.

## S2X24    **EPR SPECTRA OF POWDER SAMPLE Cu(imid)$_4$SO$_4$**

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The powder samples of metal-organic complex Cu(imid)$_4$SO$_4$ is studied by EPR. In case of a powder sample the spectrum represents a superposition of spectra of large number monocrystal particles which are chaotically oriented relatively a direction of an external magnetic field. Spectrum has a form of an absorption band placed a rather wide range of fields. It was found that for T>6 K the absorption band form was typical for rhombical anisotropy. At temperatures T<6 K the form of absorption band changes and displays unusual low-field second peak. The reasons of such behavior are discussed. The covalent bonds, Jahn-Teller effect and clusters formation will be examined.

S2X25  **TWO MAGNETIC PHASES IN LaCo$_{0.5}$Mn$_{0.5}$O$_3$ PEROVSKITE**

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The crystal structure and magnetic properties of polycrystalline LaCo$_{0.5}$Mn$_{0.5}$O$_3$ were studied by neutron powder diffraction and magnetization measurements. These studies have revealed the existence of two different crystallographic and magnetic phases in the sample. We believe low temperature ($T_C \approx 167$ K) anomaly is determined by the phase in which $3d$ ions are crystallographically disordered, whereas high temperature ($T_C \approx 207$ K) peak corresponds to the ordered phase. Ordering of the Co$^{2+}$ and Mn$^{4+}$ ions transforms O-orthorhombic ($Pbnm$) phase to monoclinic ($P2_1/n$ with a $\beta \approx 90^o$) one, and gives FM Co$^{2+}$–O–Mn$^{4+}$ exchange interactions. However, ionic disorder creates clusters with AF Mn$^{4+}$–O–Mn$^{4+}$ and Co$^{2+}$–O–Co$^{2+}$ interactions. We assumed that intrinsic chemical and structural inhomogeneities lead to a magnetic phase separation.

S2X26  **ESR studies of a quasi-tetrameric compound**
**[Cu$^{II}$(en)$_2$(H$_2$O)][Cu$^{II}$(en)$_2$Ni$_2$Cu$_5^I$(CN)$_{10}$]·2H$_2$O**

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Numerical studies of an individual tetramer in magnetic field were performed and explain the main features of experimentally observed electron spin resonance (ESR) spectra. A double-peak character of resonance lines below 15 K can be ascribed to the superposition of the transitions characteristic for an individual tetramer with $S$=0 ground state and exchange interaction about 1 K. At higher temperatures the shape of resonance lines converges to a simple one-ion $S$=1/2 state as a result of breaking intratetramer correlations.

S2X27  **Magnetic states of MgCo$_2$ and CaCo$_2$ with Laves phase structures**

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It has been observed that MgCo$_2$ has a hexagonal (C14-type) Laves phase structure, while CaCo$_2$ shows a cubic (C15-type) Laves phase structure. Both compounds are ferromagnetic in low temperature. In this paper, electronic structures for these compounds are calculated for both lattice structures of the C15-type and C14-type in the self-consistent LMTO-ASA. A gga correction is taken into account. For MgCo$_2$, the calculated total energy is shown to be minimum in the ferromagnetic state with the hexagonal C14-type structure. An antiferromagnetic solution is also obtained, but the total energy is shown to be higher than that for the ferromagnetic state. For CaCo$_2$, the total energy is minimum in the ferromagnetic state with the cubic C15-type structure. The ferromagnetic state is also obtained in the C14-type structure. However, the energy is found to be a little higher than that in the C15-type structure. The present calculated results are found to be consistent with the observed results.

S2X28 **MAGNETIC TRANSITIONS IN Ru 1222 SUPERCONDUCTING PHASE**

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$RuSr_2Gd_{2-x}Ce_xCu_2O_{10-y}$ [x = 0.6] (Ru - 1222) is a very intriguing compound where superconductivity and magnetism coexist. The temperature where the magnetic ordering occurs is much higher than the superconductive transition temperature (respectively about 175 K and 45 K) [1]. The dependence of the magnetic susceptibility on the temperature is complex. Usually the main features are interpreted assuming that the ground state is antiferromagnetic with a weak ferromagnetic component [2]. Particularly Ru - 1222 is thought to be paramagnetic over about 175 K and antiferromagnetic in the range between 175 and 80 K. Below this temperature, also a ferromagnetic ordering occurs. Anyway, not all the features of the magnetic measurements of this material can be explained in this way. Moreover, the synthesis of single phase Ru-1222 is particularly complex and some doubts remain on the proper magnetic effect of the true Ru - 1222. We point out the large spread of magnetic results in literature [2, 3, 4, 5]. Above all, we report that in the initial steps of the process also $RuSr_2GdCu_2O_8$ (Ru - 1212) form, because of the relatively low reactivity of $CeO_2$ (one of the precursor). Moreover, the relative ratio between Gd and Ce can change from point to point in Ru -1222. All these phases are magnetic and their contribute can be important in the general magnetic behaviour of the system.

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S2X29 **Magnetism of Fe clusters embedded in Co**

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We have calculated spin and orbital moments for Fe clusters of a size range of 9 to 701 atoms embedded in a Co matrix. The calculations have been carried out with a self-consistent real space LMTO-ASA method using the recursion method and we have made a comparison with earlier experimental studies. For Fe atoms close to the Fe-Co interface, the spin moments increase while atoms far from the interface exhibit more bulk like moments. The Co moments remain essentially unchanged. With increasing cluster size, the mean moments decrease due to decreased surface to volume ratio. The orbital moments of both Fe and Co stays almost constant regardless of cluster size. Our results for spin moments agree with experimental data but the orbital moments are underestimated. Small Fe clusters surrounded by Co show higher averaged total moments than bulk and multilayer systems do for a similar concentration.

S2X30 **EPR detection of the magnetic field on the surface of a single crystal of the molecule magnet $Mn_{12}$-acetate**

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EPR technique has been used as a method for measuring magnetic field and magnetic field gradient on the surface of a single crystal of the nanomagnet $Mn_{12}$-acetate. As the EPR probe we used fibrous needle of the organic conductor NMP-TCNQ. The splitting and the shift of the resonant lines of the probe at different orientation of the single crystal in the magnetic field was measured in the temperature range 300-5K. The shifts of the lines yield the magnitude of the additional magnetic field of $Mn_{12}$-acetate. In conjunction with electron microscopy, the shifts yield the magnetic field gradient at the crystal surface as a function of the temperature. The dynamic properties of detected local field have been examined at the $\mu s$ time scale by employing Pulse EPR in the low temperature interval.

S2X31 **Magnetic normal modes in nano-particles**

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We present a method to calculate the magnetic normal modes of a ferromagnetic nano-particle. The method is a hybrid of micromagnetic simulations and a dynamical matrix approach. We use the method to calculate the normal modes of a 116x60x20 nm Fe parallelepiped, in external field applied in the direction of the long axis. We find two families of spin modes which exhibit, at least to first approximation, standing-wave character with wavevector parallel and perpendicular to the applied field, respectively. With reference to film excitations, the former are assigned as backward-like, the latter as Damon-Eshbach-like modes. In addition, spin excitations localized at the particle ends, in the direction of the applied field, are found. We also observe hybridization effects, which limit the validity of the over-simplified standing-wave picture.

S2X32 **EXPERIMENTAL STUDY OF MAGNETOCALORIC EFFECT IN DIPOLAR SPIN ICE $Dy_2Ti_2O_7$**

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The magnetocaloric effect of dipolar spin ice $Dy_2Ti_2O_7$ was experimentally investigated in the temperature range 0.28 K - 8 K and in the magnetic field up to 2 T. The field induced adiabatic temperature change above 1 K can be well described using the temperature and magnetic field dependence of the magnetic entropy as calculated from the magnetic specific heat data. Cooling during the adiabatic demagnetization below 1 K can be attributed to the change of the residual entropy caused by magnetic field. The results of the demagnetization at various sweeping rates suggest that $T_{min} \approx 0.25\ K$ might represent the lowest temperature obtainable by the demagnetization of $Dy_2Ti_2O_7$.

S2X33 **Photothreshold of the group III-VI layered semiconductors**

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The photothreshold correction arisen from electronic relaxation has been calculated for the group III-VI layered semiconductors. The approach suggested formerly for metals (Volkov et al, 1995) and diamond-like semiconductors (Bechstedt et al, 1984) is used. In order to take into account the band structure and anisotropic dielectric permeability of the layered semiconductors, the calculation procedure has been modified. The valence-band wavefunctions found by Nikanishi et al (1982) are used. Results of the calculation are compared with experimental data. A large discrepancy between one-electron tight-binding theory predictions and experimental observations of photothreshold is essentially removed. The best agreement is obtained for GaSe.

S2X34 **The Problem of stoichiometry Deviation Towards Non-Metal Component in ZnS, and Native Acceptors in It**

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To study the role of surrounded atmosphere in p-doping problem of ZnS the thermodynamical analysis for ZnS (crystal) S2 (vapor) system was performed. Basing on the results of the analysis in order to obtain native defect hole conductivity in ZnS two methods method of implantation by S ions, and annealing under gold layers is suggested and realized. High-ohmic p-type samples are obtained. Two acceptor centers with thermal activation energies 0.57eV and 0.14eV were observed in p-type samples obtained by both methods. In the PL spectra of p-type samples 520nm and 345nm bands were increased.

S2X35 **Millisecond decay of free electron photoluminescence in direct-gap III-V semiconductor compounds: magnetic resonance studies**

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We report a very long non-exponential millisecond-scale decay of the non-stationary band-to-acceptor photoluminescence (PL) in pure GaAs and direct-gap AlGaAs and InGaAs alloys at low temperatures, which contradicts the accepted recombination model. We suppose that repeated trappings and releases of free electrons by shallow donors control the PL decay. To assess experimentally the role of shallow donors we have studied the kinetics of acceptor PL under a resonant excitation of neutral donors by far-infrared laser radiation in a magnetic field. We have found that the decay of band-to-acceptor PL varies strongly at $1_0$-$2p_+$ donor resonance. This confirms the proposed donor-controlled electron recombination model in GaAs and related direct-gap compounds.

S2X36 **The role of magnetic-impurity states of short-range potential in the conductivity of electron gas**

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The problem of the Landau electron scattering in the band N with an arbitrary moment by a small radius center of arbitrary depth is solved (Andreev, S.P. and Pavlova, T.V., 2004, Laser Physics, 14, 174). It is shown that the poles of the derived scattering amplitude determine a spectrum of bound and quasibound magnetic-impurity (MI) particle states. The behavior of the MI levels with m=0 in different Landau bands is investigated in details as a function of an individual impurity potential depth and magnetizing force. The explisit formula for conductivity of the gas of electrons, scattering by chaotically distributed centers in quantizing magnetic field is derived with a help of the obtained wave functions. The transverse conductivity dependence on the longitudinal electron energy, magnetizing force H and scattering length is investigated. The connection of the conductivity field dependence with the character of the spectrum of MI states is analyzed.

S2X37 **Spin Transport via Surface Acoustic Waves in GaAs Quantum Wells**

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Spin transport in semiconductor structures is typically performed in the ballistic regime with very little control of the microscopic movement of the carriers. In this contribution, we detail a microscopic photoluminescence (PL) study of spin transport using surface acoustics waves (SAWs) in a GaAs/AlGaAs quantum well. The SAWs transport the electronic spin carriers with the SAW propagation velocity within a well-defined channel determined by the SAW beam width. The photogenerated electrons and holes are spatially separated by the piezoelectric potential of the SAW resulting in a dramatic increase of the spin polarized PL signal. At remote distances up to 10 microns, the transport of spin polarized carriers is an order of magnitude larger than can be seen from simple carrier and spin diffusion. We will discuss the spin scattering mechanisms during transport and propose techniques to improve the long range transport.

S2X38 **Modelling of the platinum gettering by a porous Si layer created by hydrogen ion implantation**

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The platinum gettering phenomena in Si wafers with a void-enriched region created by hydrogen ion implantation have been considered by computer modelling. Since platinum is a lattice impurity in silicon, a mechanism for its gettering has been proposed assuming Si interstitial injection in the course of the gettering anneals, from the void-enriched layer, as a result of the surface shrinkage. This injection has been demonstrated to exponentially decrease with the annealing time. The characteristic parameters of Si interstitial injection have been found comparing the results of calculations with the published experimental data on the time dependence of platinum consentration in Si wafers for two temperatures of anneals.

S2X39 **Electrical characterisation of semiconducting thin films**

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Binary Nitides are intersting compounds that display a wide range of physical and chemical properties. Compounds such as BN,AlN etc have been well investigated. On the other hand metal nitrides like $Si_3N_3$, $Cu_3N$ and $Ni_3N$ have not been investigated to that extent. In particular $Cu_3N$ compounds are of great interest which decompose with the metals which suggests that they can be used in metallisation process which could be of great help for electronics industry. Thin films of $Cu_3N$ were prepared using dc magnetic sputtering. Van der Pauw method was used to study temperature dependence of resistivity from 10 to 300K. The activation energy was determined from the resistivity data and was obtained as 0.207 eV.

S2X40 **Surface Phonon-Polaritons on Layered GaSe Crystals**

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The spectrum of surface vibrations on GaSe exited by the optical method of attenuated total reflection (ATR) has been studied theoretically. The ATR spectra have been calculated for the geometry when the normal to the crystal surface is perpendicular to the cleavage plane. The frequency-wavevector dispersion determined by positions of the ATR spectrum minima at various angles of incident light within frequency range $214 < \nu < 254 \; cm^{-1}$ consists of two branches. The lower branch ($\nu < 245 \; cm^{-1}$) corresponds to the surface mode of type I (real mode) or type II (virtual mode) depending on the wavevector value. The upper branch ($\nu > 245 \; cm^{-1}$) corresponds to the type II surface mode. The results of the calculation have been compared with experimental data obtained by other methods. The calculated dispersion relation at small and large values of the wavevector agrees with experimental data of infrared and Raman spectroscopy.

S2X41 **Application of method of projective representations for analysis of energy spectra of elementary excitations and their dispersion in tetragonal crystals $ZnP_2$ and $CdP_2$**

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Dispersion of elementary excitations in several directions of wave vector was analysed in isostructural strongly gyrotropic enantiomorphuos tetragonal crystals $ZnP_2$ and $CdP_2$ by method of projective representations of wave vector groups. The following points of Brillouin zone were taken into consideration: $\Gamma$, $\Lambda$, Z, S, A, V, M, $\Sigma$, R, X, $\Delta$, W and U. Selection rules for different types of transitions were calculated. It was determined, which of examined points of Brilloiun zone are points of zero slope and points where dispersion curves of energy states have extremum by $\vec{k}\vec{p}$-method.
The mentioned theory method was applied to interpretation of photoluminescence, edge absorption and Raman polarized spectra, which were recorded at temperature 1.7 K.

S2X42 **Electronic structure and electric-field-gradients distribution in $Y_3Al_{5-x}Sc_xO_{12}$ : an *ab initio* study**

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The pure yttrium aluminum garnet $Y_3Al_5O_{12}$ (YAG) as a prototype of a family of rare-earth garnets with exceptional optical, mechanical, and thermal properties has been intensively studied experimentally and theoretically as well. Because of the complicated crystal structure the first correct ab initio quantum-mechanical calculations of its electronic structure were realized only recently within the OLCO-LDA-DFT approach. In this contribution, the periodic and cluster Hartree-Fock (HF) methods have been applied to investigate the electric-field-gradient (EFG) distribution in mixed $Y_3Al_{5-x}Sc_xO_{12}$ garnets. For $x = 0$, the periodic HF calculations result to the YAG crystal is more ionic than, for example, $A_2O_3$. The EFG in the both Al sites is well described within the band HF calculations. However, the influence of the Y ions on the EFG in the $Al_{oct}$ site seems to be more important. The cluster approach leads to a good agreement with experimental EFG for $Al_{tetr}$, but underestimates the EFG value at $Al_{oct}$. The influence of the cluster size and basis set choice on the calculated parameters at both Al sites was studied. For chosen basis set and clusters, the EFG tensor in $Y_3Al_{5-x}Sc_xO_{12}$ assuming possible models of Al substitution by Sc was calculated.

S2X43 **Electronic and vibrational properties of Ga(As,N) and Ga(P,N)**

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In III-V semiconductors such as GaAs and GaP, N atoms form isoelectronic impurities due to the large differences in size and electronegativity. We present a comparative study of the electronic properties and the lattice vibrations of Ga(As,N) and Ga(P,N) epitaxial layers with different N contents up to a few percent with Raman spectrosopy, photoluminescence spectroscopy, excitation spectroscopy and modulation spectroscopy. In both materials, the evolution of a GaN-like local vibrational mode and an intensity increase of forbidden Raman scattering are a manifestation of the impurity character of nitrogen in these alloys. Although the corresponding binaries of the two compounds (GaAs and GaP) differ considerably with respect to their bandstructure (GaAs: direct gap, GaP: indirect gap), both of them exhibit a coexistance between localized N-related states and extended band states. Differences between both materials arise from the fact that the N-levels in GaAs are hidden in the conduction band while in GaP they are located in the band gap.

S2X44 **Stable fourfold configurations for small vacancy clusters in silicon from ab-initio calculations**

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Using DFT calculations, we have identified new stable configurations for tri-, tetra-, and penta-vacancies in silicon. These new configurations consist of combinations of a ring-hexavacancy with three, two, or one interstitial atoms, respectively, such that all atoms remain fourfold. As a result, their energies are lower by 0.6, 1.0, and 0.6 eV, respectively, than the "part of a hexagonal ring" configurations, believed up to now to be the lowest-energy states [1, 2]. Electronic structure calculations show that, like the simple ring-hexavacancy, fourfold vacancy clusters have no energy levels in the band gap, making them optically inactive. The formation of fourfold trivacancies could resolves the disagreement between positron annihilation and IR spectroscopy data reported in [3].
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S2X45 **Threading Dislocation Density in PbTe/CaF$_2$/Si(111) thin films: symmetrical diffraction**

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We present analysis of diffuse x–ray scattering from PbTe/CaF$_2$/Si(111) thin films. Due to large lattice constant mismatch between Si substrate and CaF$_2$/PbTe large concentration of misfit and threading dislocations is expected [1]. Burgers vector is oriented along 110 direction. This implies, that for (111) plane the threading dislocations are *inclined* with respect to the surface. Intensity of diffusively scattered radiation was simulated within the Krivoglaz theory [2]. Displacement fields from threading and misfit dislocations were computed according to formulas published by Shaibani and Hazzledine [3].

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S2X46 **Metastable crystalline and amorphous tetrahedral ternary solid solutions between Ge, GaSb, and InSb: Structure and elasticity .**

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' We present the systematic study of the structure and elastic shear G and bulk B moduli in metastable crystalline and amorphous ternary solid solutions $(GaSb)_{1-x}Ge_{2x}$, $(InSb)_{1-x}Ge_{2x}$, and $(GaSb)_{1-x}(InSb)_x$ with compositions varied over all concentrations of components. The basic idea to synthesize these metastable systems in bulk forms is the complete solution of the components at high temperatures in the high-pressure (at 8 to 9 GPa) phase states with subsequent solid-state amorphization upon compression. The crystalline GaSb-Ge solid solutions are in turn obtained by room-pressure crystallization of the corresponding amorphous compounds before their decay into eutectic mixtures. The unique property of the whole synthesized set of samples is controllable variation of chemical and topological disorder in tetrahedrally bonded semiconductors.

S2X47 **Raman studies of disorder effects in electron-irradiated GaP and CdS**

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MeV-electron irradiation of semiconductors basically results in formation of primary defects, which can form complexes or clusters. Radiation-induced lattice disorder is not only revealed directly in phonon spectra, but can also affect the density of electron states.
Here we report on Raman studies of GaP and CdS irradiated at room temperature with 10-MeV electrons (fluences $\Phi$ up to $7 \times 10^{18} cm^{-2}$). In heavily-irradiated GaP additional maxima at 100 and 220 cm$^{-1}$ whose intensity increases with $\Phi$, are attributed to disorder-activated TA and LA phonons revealed due to the selection rules relaxation.
In case of Raman resonance with direct-gap (GaP) or intense donor-acceptor pair-related luminescence (CdS) a disorder-induced increase of LO phonon scattering is observed. At the resonance with a narrow exciton luminescence band (CdS) the increase of 2LO maximum is even higher due to the increase of exciton formation probability and lifetime.

S2X48  **Spin relaxation measurements in bulk CdTe at room temperature**

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The information transfer using a spin of the electron is a heart of a new technology called spintronics, where the room temperature spin relaxation time directly determines the information survival. So far, the measurements of spin dynamics in semiconductors have focused mainly on III-V semiconductors with GaAs as a typical model material. In this paper, we report on the room temperature spin relaxation measurements in bulk CdTe. We investigated the spin relaxation of the electrons by performing ultrafast laser polarization-resolved pump-probe experiments (in both the transmission and reflection geometries). We found that in CdTe and GaAs, both having a very similar band structure, the measured spin relaxation times are very similar and reach the value of about 80 ps. We concentrated also on the role of particular sample properties (doping concentration, concentration of defects, ...) and the laser excess energy (hf-Eg) on the spin relaxation time.

S2X49  **RADIATIVE ELECTRONIC STATES IN CdS POLYCRYSTALLINE LAYERS**

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The absorption spectra, in the fundamental absorption wavelength region, and the photolumines-cence of CdS thin films, components of CdS/CdTe photovoltaic cells have been studied. The pho-toluminescent spectra is dominated by the radiative band of excitons attached to the defects of crystalline lattice and to the integral impurity band, which consists of 2-3 elementary bands. The correlation between the energy spectrum of the localized states and layers thickness and annealing regime in the presence of $CdCl_2$ was established. The energies of the recombination levels in CdS films and their diagram in thermally treated films have been determined from absorption and photolumi-nescent spectra. The correlation between the short-circuit photocurrent and the structure of energy states localized in the band gap of CdS films.

S2X50  **Reflection/transmission at the rough interface of dissipative medium**

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The influence of small roughness on the reflectance/transmittance of light in solar cells has been analyzed in the first order of the perturbation theory in Green function formalism. The spectral dependencies of these values for rough semiconductor surface were calculated and compared with an experimental data obtained at the GaAs substrate. The transmittance increase by about a few percents for nanorelief roughness has been demonstrated, that agrees with experimental data for the surface-barrier photocurrent with non-smooth interface. Experimental measurements of specular, diffuse and total reflection light spectra ($\lambda$=0.4-1.0$\mu$m) have been realized for flat and different microrelief surface of GaAs substrate. The results obtained were compared with the usual scalar diffraction theory based on Kirchoff's approximation: $R_{spec} = R_0 \exp[-(4\pi\sigma n/\lambda)^2]$, $R_0 = R_{spec} + R_{diff}$ is the reflectance of a flat surface, $\sigma$ is the rms roughness (from AFM data), $\lambda$ is the wavelength and $n$ is the refractive index of surrounding medium.

S2X51 **Dynamical exchange effects in a two-dimensional many-polaron gas**

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Using a variational approach, we investigate the influence of dynamical exchange effects on the response properties and the static properties of a two-dimensional many-polaron gas. Dynamical exchange effects are not manifested in the random-phase approximation (RPA) that is widely used in the analysis of the many-polaron system. They are taken into account using a dielectric function derived in the dynamical exchange decoupling formalism. At weak electron-phonon coupling, we find that these effects lead to substantial corrections to the RPA results for the ground state energy, the effective mass, and the optical conductivity of the polaron system. Furthermore, we show that the reduction of the spectral weight of the optical absorption spectrum at frequencies above the longitudinal optical phonon frequency, due to many-body effects, is overestimated by the RPA.

S2X52 **The influence of the annealing sequence on electrical junctions observed by scanning capacitance microscopy**

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Scanning capacitance microscopy (SCM) has been widely used to examine the electrical junction profiles of silicon-based devices. The junctions in the devices are usually formed by rapid thermal annealing (RTA) or spike annealing (SA) at high temperature. Due to the photoperturbation effects, there are many difficulties in employing SCM to study the subtle correlations between electrical junctions and annealing conditions. Using low-photoperturbed SCM, operated under the same photoperturbation levels, we have observed the electrical junction narrowing produced by post-SA and -RTA furnace annealing at low temperatures. The experimental results indicate that the electrical junction formed by RTA and SA is unstable. The physical mechanism and the stability of electrical junctions formed by high temperature processes will be discussed.

S2X53 **The model of short-range inelastic electron-polar optical phonon scattering in Cdx Hg1-x Te**

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The short-range interaction potential of an electron with polar optical phonons is find by the way of solution of a Poisson equation in the limits of one unit cell. Thus the unit cell is substituted by a sphere of effective radius R=Z a (a - lattice constant) the magnitude of which lies within the limits from half of the smaller diagonal up to half of the larger diagonal of a unit cell. A comparison of the theoretical temperature dependences of electron mobility was made with experimental data for the crystals with compositions x = 0.08-0.17.The theoretical curve calculated on the basis of short-range interaction potential well agree with experimental data in the temperature range T =120  300 K whereas the curves calculated on the basis of standard long-range model differ from experiment in 1.9 -3.8 times.

S2X54 **The role of recombination processes in Seebeck effect application of Gurevich theory on Cd1-xZnxTe**

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The lifetime of carriers represents an important parameter of radiation detectors which is characteristic for them. We have focused on lifetime determination from common experiment performed on p-Cd0,96Zn0,04Te temperature dependence of Hall and Seebeck effect and electrical conductivity. The evaluation of our experiments was done on the basis of the new theory of Yu. Gurevich et al. We intend to measure photoconductivity on our samples CdTe and to compare the measured and calculated values of lifetime.

S2X55 **Photoluminescence properties of $PbI_2$ samples prepared by direct synthesis and by precipitation followed by zone melting**

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Lead iodide ($PbI_2$) belongs to promising materials for radiation detectors operating at room temperature. Samples prepared by direct synthesis and by precipitation followed by zone melting have been characterized by low-temperature photoluminescence (PL) spectroscopy. The influence of admixture of rare earth elements (REE) on the quality of prepared material has also been investigated. The observed radiative transitions in measured $PbI_2$ samples could be grouped into two cathegories: band-edge (BE) transitions at about 2.49 eV and free to shallow acceptor levels (F-B) related transitions at 2.46, 2.43, 2.38 eV. The high energy band (BE) exhibits superlinear behaviour with increasing excitation power and results from the decay of excitons. Phonon assisted transitions associated with exciton recombination as well as with shallow defect level, and involving 5-8meV LO phonons, have been observed. Application of zonal melting or REE addition within direct synthesis leads to the narrowing of spectral bands and appearance of fine spectral features, characteristic for pure material, low in defects.

S2X56 **Investigation of N Induced Changes in Photoluminescence Properties of GaInNAs/GaAs Heterostructures**

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N induced changes in photoluminescence (PL) properties of GaInNAs/GaAs heterostructures have been studied. PL spectra were taken at room temperature and 70K. Comparing the PL spectra of GaInNAs/GaAs with GaInAs/GaAs, N effects were extracted. At room temperature no PL emission was detected from N free sample, however, a weak PL emission was detected from N containing samples. As predicted in the literature, N incorporation into GaInAs causes red shift in PL spectra and broadens the peaks. Other effects influencing PL spectra of GaInAs/GaAs structures such as strain effect and the indium concentration were briefly discussed.

S2X57 **Effect of temperature on the photoluminescence properties of GaInNAs quantum well**

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The temperature dependence of photoluminescence (PL) properties of GaInNAs single quantum well (QW) has been studied. PL measurements were carried out from 70 to 300K. PL spectra reveal that the spectrums are made up of more than one peak. The peak appearing at 1205 nm at room temperature shifts to 1066 nm at 70K. This is interpreted due to a shift of PL spectra from the localized-like state to the delocalized-like state of the GaInNAs QW's e1-hh1 transition.

S2X58 **Investigation of p-type ZnO Layers Treated by RBQE method**

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One of the topical problems of optic electronics is to obtain and study the wide-band II semiconductors. The ZnO sample was implanted by S ions. n- type high ohmic ZnO samples were obtained by heat treatment in molecular oxygen atmosphere. In photoluminescence (PL) spectra of ZnO crystals new line was observed. In our opinion this line connected with the inclusion of S ions. In order to obtain p-type ZnO samples we carried out the following experiment: n-type ZnS monocrystals was treated by Radical Beam Quasi Epitaxy (RBQE) method in the atmosphere of activated oxygen obtained by RF-discharge. According to the experimental date new quasiepitaxial p-type ZnO layers were obtained. In PL spectra of new ZnO layers peaks related to sulfur have not been observed. Thus, we can conclude that during RBQE, transition of sulfur in the new epitaxial layers of ZnO does not take place.

S2X59 **Thermal Conductivity of Isotopically Enriched $^{28}$Si: Revisited**

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The thermal conductivity $\kappa$ of isotope enriched $^{28}$Si (enrichment $\geq$99.9% ) was redetermined by high precision experiments on a total of four samples of different shape and degree of isotope enrichment with particular emphasis on the range near room temperature. The results obtained in the three different laboratories are in good agreement with each other. They indicate that at room temperature $\kappa$ of $^{28}$Si exceeds $\kappa$ of Si with a natural, unmodified isotope composition by 10$\pm$2%. This finding is in disagreement with an earlier report T. Ruf *et al.*. $\kappa$ of Si with natural isotope composition is consistently found to be 2-3% lower than the values reported in the literature.

S2X60 **First-principles investigation of the electronic and optical properties of half metallic semiconductor materials: TiGaX, X=As or P**

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Using quantum mechanic calculations, band structures properties and optical transitions for novel photovoltaic materials have been studied. We have proposed, using accurate Density Functional Theory ab-initio calculations, several alloys semiconductors containing a transition metal atom of the type: TiGaAs, TiGaP, that present an isolated half metallic intermediate band (MIB) and both direct and indirect band-gaps in their structures. Recent Exact Exchange calculations confirm the existence of the MIB.

Spin polarized calculations carried out on these materials present in some of them large spin-polarization at the Fermi energy level.

To present the optical transitions characteristic of this type of intermediate band solar cell, we use the wave functions already calculated for the transitions matrix elements and phonon dispersion curves determined also by quantum mechanic calculations.

S2X61 **Synchrotron Radiation Renninger Scan in the Structural Characterization of Ion Implanted GaAs**

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Renninger Scan ($\phi$-scan) using synchrotron radiation at Brazilian Laboratory (LNLS) was used to analyze the defects in the crystalline lattice of GaAs(001) when submitted to implantation of Si ions at several doses (50 keV). X-ray rocking curves ($\omega$-scan)showed implanted regions under different strains and the amorphization limit ($7x10^{14}$ions/cm$^2$) as a function of the ion implantation dose. In the (002) $\phi$-scan, contributions from special extremely asymmetric reflections (111) (diffracted beam propagates along the crystal surface) appear as Bragg-Surface Diffraction (BSD) peaks. They allowed to determine parallel lattice parameter as well as crystalline perfection at the GaAs surface (in-plane mosaic spread) for each implanted region. Comparison between GaAs wafer and annealed samples shows the effect of residual strain (in both perpendicular and parallel directions) caused by lattice ions activation also clearly observed in the mapping of BSD peak ($\omega$:$\phi$-scans).
Support: FAPESP, CNPq, LNLS (Brazil)

S2X62 **On radiation stability of devices on the base of Si-rich SiGe alloys**

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Well known isovalent impurities increases the radiation stability of semiconductors. Most experimental and theoretical investigations performed on diluted $Si_{1-x}Ge_x$ alloy (x<0.02). The Ge atoms in $Si_{1-x}Ge_x$ alloy are the centers of annihilation of primary radiation defects. As a result in electron irradiated $Si_{1-x}Ge_x$ the concentration of divacancies $N_{V2} \sim 1/N_{Ge}^2$.
In work the radiation stability of p-n junction on the base of $Si_{1-x}Ge_x$ with 0<x<0.2 is investigated.The theoretical analysis has shown, that in this case $N_{V2} \sim 1/N_{Ge}$. The experimental data on spectral characteristics of electron irradiated p - n junctions are presented.

S2X63  **Optical properties of quaternary ZnxCdyHg1-x-yTe alloys investigated by fine structure far-IR reflectivity with Infrared Synchrotron Radiation**

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Far-infrared reflectivity spectra of different ZnxCdyHg1-x-yTe quaternary alloys were measured using infrared synchrotron radiation at the DAFNE-light facility of the INFN-LNF (Frascati, Italy). Epitaxial layers of the investigated alloys were obtained on CdTe substrates by liquid phase epitaxy at the Ioffe Institute (St. Petersburg). Experiments were performed in vacuum using a modified Bruker Equinox 55 FTIR interferometer as a function of temperature in the range from 40 K to 300 K. The spectra, measured with a resolution of 1.5 cm-1, were processed with standard Kramers-Kronig analysis to obtain the imaginary part of the dielectric function and then unfolded into a set of Lorentzian oscillators. For two samples of ZnxCdyHg1-x-yTe (x=0.05, y=0.23 and x=0.12, y=0.13), the reflection spectra show a large temperature modification and the fitting procedure yields a total of twenty-four lines. Fifteen lines have been correlated to the ternary spectral contributions of the different components CdHgTe, ZnHgTe and CdZnTe [1]. References:[1] B.V. Robouch, A. Kisiel, J. Konior, J. All. Comp. 339, 1 (2002).

S2X64  **Photoluminescence mapping of p-type to n-type conversion in CdTe by annealing in Cd atmosphere**

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Effects of annealing CdTe crystals in cadmium atmosphere are investigated simultaneously by low temperature photoluminescence and conductivity measurements. We show that undoped CdTe crystals can be easily converted from p-type to n-type material at least at the surface of the sample. Photoluminescence from the non-converted central part of the sample is only slightly modified compared to the as-grown crystal whereas photoluminescence from the remaining volume shows drastic reduction of bound excitons on shallow acceptors substituting on the cadmium sublattice. A model using fast migration of silver, copper and sodium acceptors in tellurium rich CdTe is developed to explain observed changes of electrical and optical properties.

S2X65 **Structural and electronic properties of carbon nitride and phosphide**

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$C_3N_4$ has been extensively studied, both theoretically and experimentally, due to its hardness and wide band gap. In contrast, little is known about $C_3P_4$. Based on the fact that both $C_3N_4$ and $C_3P_4$ are group IV-V covalent compounds, and $C_3P_4$ can be obtained simply by substituting N for P in $C_3N_4$, it is reasonable to believe that $C_3P_4$ may also have high bulk modulus and wide band gap. From the trend analysis of the electronic structures of group III nitrides and phosphides (particularly BN, BP, AlN, AlP, GaN and GaP) carbon phosphide may be expected to be a wide gap semiconductor with $E_g > 2$ eV.

We have investigated the stability of various possible structures for hypothetical carbon phosphide solids with composition $C_3P_4$ using first-principles calculation based on the density functional theory and the pseudopotential method. It was found that unlike $C_3N_4$, pseudocubic-$C_3P_4$ is energetically favored relative to the $\alpha$ and $\beta$ phases. The pseudocubic phase is exceptionally stable with relatively high bulk modulus and high density. Our calculation predicted that phase transition from the pseudocubic phase to other structural forms is practically impossible under pressure. Furthermore, band structure calculation reveals that pseudocubic-$C_3P_4$ is metallic within LDA.

To understand the strikingly different structural and electronic properties of $C_3N_4$ and $C_3P_4$, we further carried out a systematic investigation on the compound $C_3N_{4-n}P_n$ ($n = 0, 1, 2, 3, 4$) with N gradually replaced by P. Our results show that the different properties of $C_3P_4$ and $C_3N_4$ can be attributed essentially to the difference in electronegativities of the P and N atoms relative to the C atom and the nature of bonding in the two materials.

S2X66 **The investigation of opticaly-anisotropic semiconductors ZnO by IR-srectroscopy methods in strong magnetic field**

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Due to their unique properties (high photosensitivity, high output of photo- and cathodoluminescence, existence of pyro-and piezoelectric effect, etc.) single crystals of zinc oxide belong to the base materials for optical electronic devises, which use volumetric and surface waves.

This paper dials with the investigations of heavily doped zinc oxide single crystals using nondestructive techniques of IR spectroscopy and surface polaritons in the residual rays region taking into account coupling between three vibrational subsystems, namely, electromagnetic waves, optical lattice vibrations and plasma oscillations of free charge carriers in the presence of magnetic field and free orientation of the crystal optical axis relative to the crystal surface.

It have been shown, that outside magnetic field exert influence on the electromagnetic properties of one axis semiconductors in a different way than on the electromagnetic properties of cubic semiconductors.

Thus if outside magnetic field is neither transversal nor longitudinal relative to the optical axis ZnO, then, in the case of Faraday configuration, electromagnetic waves have resonance in two different frequencies, which do not concur with neither phonon or plasmon frequency.

S2Y101 **Structural, Electrical Transport, and Magnetic Properties of a half-Heusler Compound CoTiSb**

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Electrical resistivity, magnetic properties and structural properties of polycrystalline samples of a half-Heusler compound, CoTiSb have been studied down to low temperatures. The temperature dependence of the electrical resistivity takes a gentle maximum around 100 K, but on the whole it is regarded as semiconducting. Magnetic susceptibility is almost temperature independent above $\sim$100 K. These results are in agreement with previous results. Below $\sim$100 K the magnetic susceptibility increases and exhibits Curie-Weiss behavior. Below $\sim$5 K a rather rapid decrease of the electrical resistivity is observed. No magnetic ordering is found down to 2 K. X-ray diffraction measurements have been performed in the temperature range 20-350 K. The temperature dependence of the lattice constant is normal and the structure is found to be unchanged in the investigated temperature range.

S2Y102 **Effective antireflecting diamond-like carbon coatings for Si-solar cells**

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A diamond-like carbon films with different fraction of nitrogen was deposited by CVD method onto Si-substrate from CH4:H2:N2 gas mixtures. Extinction k and refractive coefficient n of the films was defined from ellipsometric measurements in wavelength range of 0.4-0.75 mkm. In range of 0.75-1.2 mkm exponential extrapolation of n and k was used. Optimal thickness of the one-layer antireflectance coatings of Si-solar cells was calculated. Efficiency of coatings was found as a rising of photocurrent density. Dependence of photocurrent vs. thickness and parameters n and k of coatings was calculated. Best efficiency of coatings was found in accordance with highest currents. It follows that the films with best optical constants was deposited from 10

S2Y103 **SPM study of $Mn_{12}O_{12}(O_2CC_4H_3S)_{16}(H_2O)_4$ molecules on Au**

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Single-molecule magnets have become the focus of considerable interest for their noble magnetic properties and potential application to nanoscale magnetic storage devices and quantum devices. However, only a few results have been reported on forming monolayer or submonolayer films of these materials. Here we present the synthesis of $Mn_{12}O_{12}$ $(O_2CC_4H_3S)_{16}(H_2O)_4$ single-molecule magnet, a derivative compound of the well-known $Mn_{12}$ acetate, and its crystallographic and magnetic data from which we obtained the structure, spin, anisotropy constant, blocking temperature, and relaxation time of the molecule. We also present the results on the chemical deposition of the molecules on Au surface, and the mechanical and electronic properties of the molecules studied by atomic force microscopy and scanning tunneling microscopy.

S2Y104 **ANOMALIES IN THERMOPOWER OF TENSILE-STRAINED BISMUTH NANOWIRES**

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Bismuth nanowires fabricated by the glass-coated melt-spinning method allow to combine a high strength of a thin glass capillary and unique electronic properties of Bi, which has a low mechanical strength in free-standing state. These wires offer an unique opportunity for basic research of physical properties under very large elastic strains. We have investigated the influence of tensile deformations on the thermopower (TEP) of Bi/Pyrex wires with diameters 100 - 900 nm. In the unstrained state, both the sign and magnitude of the TEP depend on temperature, sample diameter and quality, however, at high strains ($> 1$ %), the TEP is negative for all the samples and reaches values from - 70 to - 90 $\mu$V/K at strains $\sim 2.6$ %. These large values are determined mainly by the strain-induced changes in the topology and total volume of the Fermi-surface. This work was supported by MRDA/CRDF (Award No. MP2-3046).

S2Y105 **Microwave-hydrothermal synthesis of nanostructured magnetic ceramics from industrial effluents**

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One of the major environmental problems related to the steel industry comes from pickling plants. Steel finishing operations such as the cold rolling, galvanizing, tin-plating and enameling of semi-finished steel involve a surface cleaning process to eliminate scale, rust and dirt. This process is carried out by immersion of steel in hot acidic solutions, mostly sulfuric or hydrochloric, which in turn creates a toxic waste containing residual acid and salts (spent pickling liquor). Pickling solutions are specifically listed as hazardous waste in many countries. The objective of this work is to produce, by the first time, magnetic materials from chloride steel pickling liquors by microwave-hydrothermal synthesis. Different conditions of temperature, time and heating rate were employed to produce magnetic materials. The powders were chemically, structurally and morphologically characterized by Ion Coupled Plasma-Mass Spectrometer, X-ray diffraction, Raman spectroscopy and scanning electron microscopy were used to characterize the powders synthesized. The results demonstrated that the microwave-hydrothermal method is a very efficient method to produce magnetic materials and also to eliminate the heavy metal contamination from the spent liquor. The efficient incorporation of these elements together with the iron in the ferrite precursor was an important outcome of the proposed process.

S2Y106 **Exciton Energies and Decay Probabilities in GaN/AlN Quantum Structures**

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In this work Electron-hole Coulomb interaction exciton energies and probabilities of their radiation decay are calculated for GaN/AlN quantum dot(QD). Plane QDs are considered and only vertical confinement is accounted. Piezoelectrostatic potential is considered in the tight binding approximation. Eigenfuncions of particles confined in rectangular potential well with finite barrier were used as a basis set for expanding the electrons and holes wave functions. Electron-hole Coulomb interaction is calculated by perturbation theory. Te probability of radiative transition of gound state excitons is very low. The probability of radiation decay significantly increases for higher energetic excitons. For 4.8nm dot size exciton energies are between 2.5 and 6 eV. Exciton density, probability of their radiative decay, and Coulomb attraction energy is maximum in 3.75  4.75 eV energy range.The picture is less pronounced for smaller QDs.

S2Y107 **Micro-Raman spectroscopy of microwave A(B1/3Nb2/3)O3 electroceramics**

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A(B1/3Nb2/3)O3 ceramics (A=Ba or Sr, B=Mg, Mn or Zn) exhibit remarkable microwave dielectric properties for use as resonators in telecommunication devices. In these materials, the optical phonons determine their dielectric response, which in turn depends on the preparation conditions. In this respect, the hydrothermal technology appears as the most promising route for environmentally friendly and low-cost production of advanced ceramics. A recent innovation in this technology was the introduction of microwaves into the reaction vessels to produce materials with different structural and morphological characteristics from the conventional powders. In this work, we report the phonon properties of A(B1/3Nb2/3)O3 powders synthesized by microwave-hydrothermal process. Oriented and large needle-like crystals were carefully produced for examination by polarized micro-Raman spectroscopy. The complete assignment of the vibrational modes as a function of chemical composition in A(B1/3Nb2/3)O3 ceramics was carried out through the analysis of the peak evolutions besides factor-group predictions.

S2Y108 **Anisotropic ab plane magnetoresistance in $Nd_{2-x}Ce_xCuO_{4+\delta}$**

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Underdoped $Nd_{2-x}Ce_xCuO_{4+\delta}$ (x = 0.12) single crystal film reveals strong angular dependence of the in - plane magnetoresistance on the orientation of the external magnetic field (B = 5T) within the ab plane. At T = 4.2K the in - plane magnetoresistance with minima and maxima alternating in $45^o$ was found. The decreasing the temperature down to 1.5K results in more than one order of magnitude rise of anisotropy magnetoresistance that underlies its low temperature nature. The effect is ascribed to peculiarities of a hole transport, that supports the two band concept of the transport in $Nd_{2-x}Ce_xCuO_{4+\delta}$. We argue the common nature of this anisotropic magnetoresistance in hole doped YBaCuO and electron doped NdCeCuO. At T = 1.5K we observed the unusual reentrant field dependence of magnetoresistance supposedly due to the ordering of Nd subsistem.

S2Y109 **Phonon breakdown in zinc in strong magnetic fields**

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The results of analysis angle and temperature dependences of magnetoresistance (MR) measurements of Zn monocrystal with orientation [1120] at T=4.2K-30K in strong magnetic fields (up to 80kOe) are represented. In the angle interval of 30-50 degrees and T=12K-20K thin structure of MR has been detected, which is not observed at 4.2K. In this temperature region a small-angle scattering of electrons on long-wave phonons becomes effective. Such scattering is inelastic, and practically in all interval of rotation angles field has a diffusive character. The thin structure of MR appears as a result of strong intersheet electron-phonon scattering under conditions of the umklapp process. By the analogy with the magnetic breakdown effect, this phenomenon is named phonon breakdown. In this case orbits of monster "sleeves" combinations must pass near the $\alpha$ needle, so the small electron orbit provides a "bridge" for the formation of new two-sheet or three-sheet temperature breakdown orbits.

**S2Y110** **Electronic transport in compacted powder of the different shape WS2 nanoparticles.**

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The pellets made of the different shape WS2 nanoparticles were the subject of the electronic transport properties (resistivity and Hall coefficient) study. The plate-like and fullerene-like shape WS2 nanoparticles were compacted and subjected to the heat treatment. The data was obtained at the wide temperature interval and the various magnetic fields using the van der Pauw technique. The results demonstrate the semiconducting behavior of the samples and the sharp distinction in the conductivity and the other parameters for the pellets compacting of the different shape nanoparticles. It can be induced by the difference in electrical contacts of the particles together with the difference in the electronic structure of the dissimilar nanoparticles.

**S2Y111** **Superconducting parameters of zero-dimensional In nanoparticles**

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A series of nine sets of In nanoparticle powders, with mean diameters covering 2 to 80 nm, has been fabricated by employing the gas-condensation method. The purity of the powder was examined by using x-ray diffraction, and the mean diameter and size distribution were determined from AFM images and x-ray diffraction profiles. Low temperature electrical resistivity, ac magnetic susceptibility, and specific heat were measured to study the effects of finite size on the superconducting parameters. A slight increase in TC, presumably due to the revealing of surface superconductivity, was evident in particles bigger than 14 nm. Huge enhancements in HC, which increases by a factor of at least two orders-of-magnitude, were observed in all nanoparticles. The superconducting coupling strength was found to increase considerably as the particle size was reduced for particles smaller than 14 nm, below which it becomes decreasing as the size was further reduced. No signs of superconductivity were observed in 2-nm In particles.

**S2Y112** **Direct determination of electron-phonon interaction in 2H-TaSe$_2$**

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In this work we continue a series of investigations aimed at clearing dark sports in the picture of electron-phonon interaction (EPI) in transition metal dichalcogenides. The first step was made by successful determination of EPI function, Debye temperature and other parameters of electron and phonon subsystems in 2T-VSe$_2$ [G.V.Kamarchuk, et al., Phys.Rev. B 63 (2001) 073107]. Here we report results obtained for the first time for EPI function of another compound of this family, namely 2H-TaSe$_2$. Experiments were carried out at liquid helium temperature with noble metals-2H-TaSe$_2$ heterocontacts using point-contact spectroscopy technique. Current-voltage characteristics of point contacts and their first and second derivatives were recorded for contacts satisfying spectroscopic regimes of current flow. This allowed direct observation of EPI and determination of its peculiarities in 2H-TaSe$_2$. This work was supported by STCU and NATO.

S2Y113 **Rapidly solidified Al-Ni-Zr alloys - microstructure and phase composition**

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The paper provides a detailed investigation of microstructure and phase composition of rapidly solidified and annealed AlNi18.5 and AlNi17Zr1.8 ribbons. The ribbons were prepared by melt spinning (planar flow casting) technique. Microstructure and phase composition have been studied by TEM and XRD. Furthermore, the specimens were annealed and subsequently subjected to microstructural investigation for an evaluation of their thermal stability. Rapidly solidified alloys are composed of a-Al and Al3Ni phase grains. No significant difference in shape between Al and Al3Ni grains was found. Al9Ni2 metastable phase was indentified in rapidly solidified AlNi17Zr1.8 alloy and Al3Zr phase precipitates from a-Al solid solution in the AlNi17Zr1.8 alloy after high temperature annealing.

S2Y114 **NON-EQUILIBRIUM MAGNETIZATION OF ELECTRON GAS IN METALS**

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It is prooved theoretically that in non-homogeneous and, generally, time-dependent external fields (electric, elastic etc.) a non-equilibrium electron magnetization of degenerate conductor appears in addition to equilibrium magnetism described by Pauli and Landau. The general expression connecting the additional magnetic susceptibility with non-equilibrium part of electron distribution function is derived. As an example, the distribution of non-equilibrium magnetization in conducting half-space under constant bias magnetic field and alternating electric voltage applied to its surface, has been found. In view of high sensitivity of contemporary magnetometry (based on SQUID technique) our estimation shows observability of the effect, at least in substances with narrow conduction band.

S2Y115 **Optical properties of carbon NT-PPV composites : influence of the PPV conversion temperature**

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Optical absorption, photoluminescence, Raman scattering spectra of carbon nanotube PPV composite films are studied as function of precursor conversion temperature in the range 120-300 C, of precursor aging and of NT concentrations. Dramatic changes are observed in all optical spectra for 120 C PPV conversion temperature with respect to those obtained for 300 C PPV. It is found that the effect of the low temperature conversion on all the optical spectra is similar to that of increasing the NT concentration in standard PPV. From the dramatic changes in the PL spectra of the different composite films, taken at 300K and 77K, we can prove that the charge migration process between segments is the more important mechanism for the energy transfer from short to long segments.

**S2Y117**  **Electron-Hole Coulomb Interaction in Stacks of ZnSe/CdSe Quantum Dots**

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In this work we investigated electron-hole Coulomb interaction in two- and three-fold stacks of quantum dots(QD) in ZnSe/CdSe system and defined exciton energies using single-particle model in a single band effective mass approximation.Thickness of QD layers was counted to be bellow the critical thickness and only vertical carrier confinement was considered. To take into account spatially varying cadmium concentration in QD Poschl-Teller potential was used as a singe-particle potential. Coupling between QDs of neighboring layers and electron-hole Coulomb interaction were considered in the framework of perturbation theory. Our calculations showed significant enhancement of exciton binding energy in two-fold stacks: for 0.6nm dot size up to 3.2 barrier thickness binding energy of excitons of lowest energy exceeds exciton binding energy in a isolated dot. In three-fold stacks binding energy reduces about 3 times.

**S2Y118**  **Curvature influence on carbon nanotube electronic structure:  modelling and photoluminescence experiments**

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The original computer programme, developed earlier for numerical calculation of electron density of states for single-wall carbon nanotubes [1], has been modified for taking into account the curvature of graphene sheet. The results of calculations have been compared with the experimental data on photoluminescence of suspensions of individual single-wall carbon nanotubes excited by radiation of Ti:saphire laser with wavelengths ranging from 700 nm to 1000 nm.

1.   A.V. Osadchy, E.D. Obraztsova, S.V. Terekhov, V.Yu.  Yurov, JETP Lett.  77 (2003) 405-410.

**S2Y119**  **Field-induced Antiferroquadrupolar Order in Antiferromagnetic $Dy_{1-x}Gd_xB_2C_2$ ($0.25 \leq x \leq 0.4$) Compounds**

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Gd substitution in $DyB_2C_2$ that undergoes an antiferroquadrupolar (AFQ) ordering at $T_Q = 24.7$ K and an antiferromagnetic (AFM) one at $T_N = 15.3$ K enhances the AFM interaction and weakens the AFQ interaction, and a transition sequence at 20%Gd is the reverse of that in $DyB_2C_2$. Magnetization and specfic heat experiments reveal that the AFQ ordered phase disappears under zero field for $0.25 \leq x$, and that field-induced AFQ order transition appears in the AFM phases for $0.25 \leq x \leq 0.4$, which is clearly observed with magnetic fields along the [1 1 0] direction in the tetragonal basal plane. Similar phenomenon has been observed in $TbB_2C_2$ that is an AFM compound with $T_N = 21.7$ K. Magnetic fields stabilize the AFQ order which coexists with the AFM order.

S2Y120 **Magnetic-entropy change in Mn1.1Fe0.9P0.7As0.3-xGex**

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We have studied the magnetic and magnetocaloric properties of Mn1.1Fe0.9P0.7As0.3-xGex compounds with x = 0, 0.05, 0.1, 0.15, 0.2 and 0.3. X-ray diffraction shows that all the compounds crystallize in the Fe2P-type structure. Magnetic measurements show that the compounds are ferromagnetic and the Curie temperature increases with increasing Ge content from 152 K for x = 0 to 380 K for x = 0.3. A field-induced first-order magnetic phase transition is observed just above the Curie temperature. The magnetic-entropy change is derived from the magnetization data by using the Maxwell relation. The maximum magnetic-entropy change observed in this system reaches about 40 J/kgK for a field change from 0 to 3 T around 270 K for the compound with x = 0.1.

S2Y121 **Influence of oxide layers on copper optical properties in a wide spectral range**

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*2)*

Our purpose is build-up a complete pattern of copper structure in a wide spectral interval, including intraband, interband and relaxation absorption. Therefore in sectional operation we have lead a spectral research copper and used model of a continuous oxide, which more responds to modern ideas about surface structure of metal. In outcome we were obtained optical constants nonoxide copper in a wide spectral range, and particular basic electronic performances of metal.
Investigated copper samples made by diamond microgrinding of massive metal also were treated in vacuum at temperature 500C for elimination residual tension and reduction in the order of a surface layer.
Primary data are the results of observed ellipometric parameters (delta) and (psi) at different angles of light incidence for several wavelengths. The measuring was carried out at a room temperature. To search solving of an inverse problem of ellipsometry for single-layer model, we determine parameters of metal an index of refraction n, index of absorption (kapa) and thickness of an oxide layer d. For an oxide layer decreasing of indexes of absorption and refractive rather essential in all investigated spectral range, and this decreasing are 30 and 70 percentage respectively.
The results obtained for nonoxide copper sample are better agreed with the theoretical calculations. The oxide layer on a surface of a copper mirror essentially influences on its optical properties, that results in distorting the data on electronic structure of this metal.
Thus, the measurement of optical constants for copper in a wide spectral range at various angles of light incidence on metal has allowed determining such characteristics of electron subsystem of this metal as mass, density and speed of electron at the Fermi surface. The values of main energy intervals in a band structure of this metal which are responsible for characteristic structure of a spectrum of the interband absorption for both oxidized and nonoxide copper sample are also determined.
The outcomes are obtained in this work, permit to lead the detailed analysis of energy structure of pure copper, and also offer a procedure of such calculations.

**S2Y122** **Characterization of electrical and structural properties of Be+ implanted InP by Raman scattering**

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Raman spectra of InP(100) implanted with 100 keV Be ions, both before and after annealing, were obtained at room temperature, in backscattering geometry, using the 488 nm line of Ar laser. The implantation-induced LO-line shape changes were observed with increasing fluences from $10^{13}$ to $10^{15} \ cm^{-2}$. We explained the modifications of the spectra via disorder-induced selection rule breakdown and estimated nanocrystallite size for different fluences according to the model of reduction of the spatial correlation length. After thermal annealing, the implanted layers recovered their crystalline structure at temperature as low as $600^{o}$C. Above this temperature the Be electrical activation was evidenced by the modification of the LO-line, which is interpreted as due to the coupling between the LO phonon and an overdamped plasmon. From the line-shape analysis we have obtained information about the electrical properties of doped InP layer.

**S2Y123** **Frequency dependent dielectric behavior of polyaniline-fly ash composites.**

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The composites of polyaniline-fly ash have been prepared with various compositions (15. 25, 35 and 45 wt percentage of fly ash taken from pulverized coal fuel fired boiler of thermal power station). We have investigated their dielectric properties in the frequency range 10E2-10E6 Hz. A large value of dielectric constant has been found. This is because of orientation polarization and tight binding force between the ions or atoms in the fly ash. The resulting composite sample is of great scientific and technological interest because of its high dielectric constant.

**S2Y124** **Magnetic Properties of CoPtW Alloys Obtained by Electrochemical Deposition**

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The magnetic properties of CoPtW alloys obtained electrochemically from aqueous solutions [1] were investigated in order to evaluate their reliability as permanent magnets.
The room temperature in plane($\parallel$) and perpendicular ($\perp$) hysteresis cycles parameters obtained for deposits prepared sequentially using the same electrolyte in two laboratories, show the possibility to obtain permanent magnets with reproducible characteristics. The 1T magnetization is $0.60 \pm 0.06 emu/mm^3$; the $\parallel$ and $\perp$ remanent magnetization and coercivities are respectively $0.27 \pm 0.03$ and $0.15 \pm 0.03 emu/mm^3$ and $0.23 \pm 0.02$ and $0.24 \pm 0.04$T. The saturation magnetization is in reasonable agreement with the estimate based on the composition of the deposits: $0.7 \pm 0.03 emu/mm^3$[2,3].
The degradation of the magnetic parameters with temperature is better than $15\%$ up to 100C. The thermal stability at 400K of the remanent perpendicular magnetization is of the order of $1\%$ after the first hour. The long term stability of the magnetic properties of the deposits during a period of at least one year is better than $10\%$.

[1]- M.Bestetti, P.L.Cavallotti, S.Franz, L.Gobbatto, J.M.Machado da Silva and M.A.Sá, Proc. Electrochem. Soc. 2001.
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S2Y125 **Structural Characterization of *GaN* Three-Dimensional Structures Grown by MOCVD Using X-Ray Diffraction**

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Novel *3D* gallium structures obtained by commercial organometallics and conventional metal-organic vapour phase epitaxy system (MOCVD) were studied by X-ray diffraction techniques. These *3D* structures grow up naturally on *Si*, *GaAs*, $Al_2O_3$, quartz, and metals substrates and their shape/dimensions depend on the growth conditions and mainly on the temperature. These mettalic structures when submitted to $NH_3$ flow at different temperatures ($650 - 750^oC$) favor the growth of *GaN* on the substrates. X-ray grazing incidence diffraction used to investigate these structures allowed to confirm the presence of the expected nitride. X-ray reflectivity has provided the characteristic fringe pattern confirming the good quality of the *GaN* growth. Furthermore, the results also allowed us to check the occurrence of a reasonable defined *C* layer on top of the substrate and responsible to keep the organization of the *GaN* structure, besides the normal information on the layer density, thickness and roughness.

S2Y126 **Unusual Low-Temperature Phase in the Al-Pd-Mn Alloy-System**

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We report the observation of an unusual spin-glass phase in icosahedral and decagonal $Al_{69.8}Pd_{12.1}Mn_{18.1}$. Contrary to the case of common spin glasses, we observe a drastic decrease of the $^{27}Al$ NMR line-width with decreasing $T$ below $T_f$. Below 1.2K, the shape of the Al NMR-spectra of both compounds is nearly identical and three times narrower than it is at the freezing temperatures that are 19 and 12 K, respectively. The nuclear magnetization recovery curves reveal the coexistence of two processes. One agrees with the expectations for a spin-glass frozen state with a large distribution of $T_1^{-1}$s, the other reveals a single $T_1^{-1}$. Our data is consistent with a gradual formation of an unknown phase with very different dynamics that grows in volume with decreasing $T$ and reaches 100% at 0.1K. Similar phenomena as the one described here have - to our knowledge - not yet been reported for any crystalline material.

S2Y127 **Properties of FeCoZr nanoclusters in aluminium oxide matrix**

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Phase composition and DC/AC conductance of FeCoZr nanoparticles in aluminium oxide with metal to dielectric ratio X=0.30-0.65 were studied. Mossbauer spectroscopy has shown that ratio of 3- and 2-fold-charged Fe ions depended on X. This could be evident of chemical elements redistribution between metallic clusters and dielectric matrix. DC conductance at 78-300 K have shown the well-known Mott or Shklovski-Efros laws. Electric measurements in the frequency range from 0.1 to 100 KHz exhibited the increase of capacitance up to 2-3 orders by magnitude at achieving some threshold value of bias voltage in the samples beyond the percolation threshold. This effect was always accompanied by the decrease of real part of impedance. The value of threshold bias voltage decreased with the growth of X in the studied composites.

S2Y128 **Pressure effect on magnetovolume properties of $Nd_5Si_{1.45}Ge_{2.55}$**

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$Nd_5Si_{1.45}Ge_{2.55}$ compound belongs to the group of intensively studied magnetocaloric $R_5(Si,Ge)_4$ compounds. It crystallizes in monoclinic structure with purely magnetic transitions at 60 K. We report a study of the effect of hydrostatic pressure up to 0.9 GPa by means of magnetization, compressibility, and linear thermal expansion measurements. The pressure-induced increase of the Cure temperature $T_C$ is rather moderate: $dT_C/dp = + 4$ K/GPa. Pressure effects on magnetization at 5 K and 5 Tesla are negligible, in agreement with localized character of the Nd moment. The value of $dlnT_C/dlnV$ calculated with the use of the measured value of compressibility ($k = 1.71 \times 10^{-2}$ $GPa^{-1}$) is nearly three times lower than that estimated from the dependence of $T_C$ on the lattice cell volume upon changing the Si/Ge ratio. It demonstrates that the dependence of $T_C$ on the Si/Ge ratio cannot be explained by a pure volume effect.

S2Y129 **Transport and magnetic properties of PbMnTe doped with Cr, Mo.**

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Doping of the lead telluride and some other narrow-gap IV-VI semiconductors with certain impurities results in appearance of a range of strong and unusual effects (such as Fermi-level pinning and persistent photoconductivity) that are not characteristic for the undoped material. The appearance these phenomena results from the valence instability of an impurity atom. In the case of the group III impurities indium and gallium, the Fermi level pinning comes up from switching of the impurity atom valence by two: Ga+ to Ga3+. For these impurities, the persistent photoconductivity is observed both when the Fermi level is pinned in the gap or in the allowed band.

The transition metal and rare earth impurities are of a special interest since the position of the respective impurity levels may be, in principle, tuned by magnetic field. In PbTe(Yb) and PbTe(Cr) the Fermi level is pinned in one of allowed bands, but the valence of an impurity atom is changing by 1: Yb2+ to Yb3+ and Cr2+ to Cr3+. In this case the persistent photoconductivity effect and other long-term non-equilibrium processes are not observed. They appear only in the doped lead telluride-based alloys, for instance, in PbMnTe, when the position of the pinned Fermi level shifts to the gap.

The impurity states that are formed by other transition metal - molybdenum - have not been studied previously.

We have investigated transport and magnetic properties of the PbMnTe alloys doped with Cr and Mo. It is known that doping of PbTe with Mn gives rise to the bandgap with the rate of 40 meV/mol%MnTe, but does not provide appearance of local or quasilocal levels in the vicinity of the actual bands.

For the PbMnTe(Cr) alloys, the Cr concentration in all samples was enough to pin the Fermi level, and for the samples with different Mn content the Fermi level could be pinned either in the conduction band or within the gap. Anomalous behavior of the pinned Fermi level position with manganese concentration was observed.

It was shown that in PbMnTe(Mo) the Fermi level could be pinned within the valence band as well as within the gap. In the latter case considerable persistent photoconductivity was observed at low temperatures.

The studies of the magnetic susceptibility showed that magnetic properties of PbMnTe doped with Cr and Mo are defined by weak antiferromagnetic interaction between manganese ions. Deviation of the temperature dependence of magnetic susceptibility of PbMnTe(Mo) alloys from CurieWeiss law was found at the temperatures higher than 100 K. The possible reasons of the effect are discussed.

S2Y130 **Epitaxial growth of the 20 nm thick-Pb(Zr0.3,Ti0.7)O3 thin films on SrTiO3 single crystal for nano-data storage application**

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Recently, much attention has been paid to the application of $SrRuO_3$ (SRO) thin films as an electrode for various electronic devices because of their high electrical conductivity, thermal conductivity, and chemical stability. SRO has a $GdFeO_3$ type orthorhombic structure with lattice parameters of a = 0.55670 nm, b = 0.55304 nm, and c = 0.78446 nm.[1] SRO is also described as a pseudocubic perovskite structure[2] with a lattice parameter of a = 0.39231 nm. Therefore, the SRO thin film electrode can be utilized as a seed layer for heteroepitaxial growth of other perovskite oxides. Particularly for ferroelectric or piezoelectric devices using perovskite oxides, heteroepitaxial growth would bring about the following advantages: increase in remanent polarization ($P_r$) by aligning the $<100>$ polarization axis in the growth direction, increase in spontaneous polarization by straining the crystal lattice along the polarization axis,[3] and increase in elastic stiffness. It has been reported that epitaxial thin films of $Pb(Zr,Ti)O_3$ (PZT) grown on SRO exhibit large $P_r$ and excellent fatigue resistance. SRO (100) epitaxial thin films can be grown on perovskite-type single crystal substrates such as $SrTiO_3$(100) and $LaAlO_3$(100). However, it is difficult to fabricate SRO(100) epitaxial thin films directly on Si substrates. In order to solve this problem, SRO/Buffer layer/Si structures have been suggested, and are being increasingly studied at present. In this study, buffer layer such as HfN has been proposed for the suppression of crystallinity at the interface between SRO films and Si substrates.

The SRO films were grown onto etched $SrTiO_3$ single crystal substrates by pulsed laser deposition (PLD) using a KrF excimer laser ($\lambda$ = 248 nm). The deposition conditions of SRO and PZT films using PLD are follows: deposition temperature of SRO and PZT are 700 and 650$^o$C, respectively. Energy density of SRO and PZT is 2 J/cm$^2$, repetition rate is 4 Hz, deposition pressure is 100 mTorr. STO was etched in a buffered $NH_4$F/-HF (pH/= 5.8) solution and subsequently annealed in $O_2$ (1000$^o$C, 30 min). The crystalline structures of the films were analyzed by x-ray diffraction (XRD, Rigaku D/MAX/-RC).

STO single crystals etched in a buffered solution had the flat terraces with straight edges in a $TiO_2$ terminated surface with a step of 0.4 nm height. Line profiles of the 10 nm thick/-SRO films grown on STO showed a step of approximately 0.4 nm height. PZT and SRO films were epitaxially grown on the treated STO substrates. The further study will be focused on the evaluation of ferroelectric properties in epitaxial PZT(20 nm)SROSTO structure.

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S2Y131 **ELECTRONIC STRUCTURE AND THE SITE PREFERENCE OF CHROMIUM IN $Fe_3Al$ ALLOY BY THE TB-LMTO-ASA METHOD**

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$Fe_3Al$ and $Fe_3Si$ alloys crystallise in $DO_3$-type structure. There are two non-equivalent types of iron with different chemical neighbourhood (A,C) and B sublattices. Transition metal atoms preferentially occupy one type of these sites depending on their position in the periodic table of elements. However, the rules seem to be not obeyed by chromium impurities at least in Fe3Si. The aim of paper is to study the site preference of Cr atoms in $Fe_3Al$ alloy and to investigate the influence of the local surrounding of iron on its magnetic moment and density of states in compound where iron is substituted by chromium Both the total and partial densities of states are analysed. Calculations were carried out with the TB-LMTO-ASA method for the experimental values of lattice parameter.

S2Y132 **Frequency dependent dielectric behavior of cadmium and chromium co-substituted nickel ferrite**

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The frequency dependent dielectric properties of $Ni_{1-x}Cd_xCr_xFe_{2-x}O_4$ (x=0.0,0.3,0.5,0.7 and 1.0) spinel ferrite system are studied by means of dielectric constant, dielectric loss and conductivity measurements at 300k in the frequency range 100Hz-2MHz. The highest value of conductivity and dielectric constant is observed for x=0.3 composition. The conductivity and dielectric constant are found to decrease with increase in frequency for all the composition, exhibiting normal ferrimagnetic behavior and is attributed to Maxwell-Wagner type interfacial polarization. The observed broadening of relaxation peak with content in dielectric loss versus frequency is due to the strengthening of dipole-dipole interactions.

S2Y133 **Magnetic and transport properties of Co-Al-O films prepared by laser ablation**

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Structural, magnetic and transport properties of Co-Al-O insulated granular films fabricated by laser ablation are reported. The films consisting of Co nanogranules embedded in an $Al_2O_3$ matrix were deposited from different $Co_x(Al_2O_3)_{1-x}$ targets. The transmission electron microscopy confirms a granular structure of films with Co grains of few nm in diameter embedded in an insulating $Al_2O_3$ matrix. The influence of deposition conditions on the film composition and the structure is studied. Then the magnetic and transport properties are investigated in a wide temperature range. Results of annealing treatment on magnetic and transport properties are presented also.

**S2Y134** **Thermoelectric properties near electron - topological transition in Te - doped Bi nanowires**

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We report the investigation of the effect of the uniaxial stretch up to 3 % on the thermopower and resistivity in Bi doped by Te nanowires with diameters between $0.2 < d < 4.0\ \mu$. Measurements of thermopower at liquid nitrogen temperatures reveal anomalies (minimum and maximum) on dependence of thermopower $S(\epsilon)$ upon applied deformation $\epsilon$ in the range $0.3 < \epsilon < 1.0$ %. A step-like peculiarity appears on the resistance dependence $R(\epsilon)$ in the same deformation range. Using an analysis of the Shubnikov de Haas oscillation frequencies on stretching we can follow the changes in the Fermi surface topology during deformation. The observed peculiarities on $S(\epsilon)$ correlate with data obtained by Shubnikov de Haas oscillations method. These correlations allow to conclude that observed peculiarities are due by Electron Topological Transitions (Lifshitz transition). This work was supported by MRDA/CRDF Award No. MP2-3046.

**S2Y135** **Study of energy levels of RE ions incorporated in matrix of lead tungstate crystal**

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The lead tungstate crystals are doped by rare earth ions in order to change their luminescent and scintillation characteristics. Physical mechanism of the effect is still under discussion. Results of our both experimental and theoretical studies of spectral properties of the lead tungstate crystals doped with the europium, praseodymium, and ytterbium ions are reported. In order to identify obtained spectral characteristics the parameterization procedure for impurity f - ions was carried out. Obtained parameters were used to solve a direct spectroscopy task: calculation of the energies of all actual in the luminescence levels of impurity ions. Noted above calculations and analysis of the Stark levels structure allowed us to do conclusion about existence of two types of the emission centers formed on a basis of the RE ions in the lead tungstate crystal lattice.

**S2Y136** **Magnetic and transport properties of $R_2NiGe_6$ ternary compounds**

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The ternary germanides with $Ce_2NiGe_6$ structure (space group Cm2m, Pirson symbol oS18) were found under systematic study of the R-Ni-Ge ternary systems. Samples were prepared by arc melting of the constituent elements in an argon atmosphere and then annealed at 870 K for 720 h. Phase analysis was carried out using X-ray patterns obtained on a Philips PW1130 powder diffractometer ($CuK_\alpha$ radiation). The magnetic measurements were carried out up to 10 T in the range 4-300 K. The electrotransport properties were measured using two-probes method. Temperature dependence of the magnetization for the $Dy_2NiGe_6$, $Gd_2NiGe_6$, $Ho_2NiGe_6$ ternary compounds in the magnetic field 0.1 T indicate on the antiferromagnetic order under low temperatures. Ternary compound $Y_2NiGe_6$ is Pauli paramagnetic.

**S2Y137** **Synthesis and characterization of SiC nanowires directly from NiO/Si**

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SiC nanowires were synthesized by direct heating NiO catalyzed Si substrate at 1000 - 1100 C. Si substrate was used as a Si source material. Carbothermal reduction of WO3/C provided carbon source and also reductive environment to produce SiC nanowires. Synthesized SiC nanowires had lengths over tens of micrometers with diameters of a few tens of nanometers. The crystallinity of nanowires was investigated by XRD and TEM, which showed cubic structure of SiC. The field emission properties of SiC nanowires were also investigated by using current density-electric field measurements. Our SiC nanowires showed low turn-on voltage for field emission and reasonable field enhancement factor. Modification of SiC nanowires was also investigated by using chemical vapor deposition and vapor evaporation methods.

**S2Y138** **Quantum confinement effect on $ZnP_2$ nanoparticles in zeolite Na-X**

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We report that for the first time the nanoparticles of II-V semiconductor ($ZnP_2$) were prepared and studied. $ZnP_2$ nanoparticles were prepared by incorporation into zeolite Na-X matrix. Absorption, diffuse reflection (DR) and photoluminescence (PL) spectra of the $ZnP_2$ nanoclusters incorporated into the supercages of zeolite Na-X were measured at the temperature 77 K. Five bands $B_1$-$B_5$ are observed in both the DR and PL spectra demonstrating the blue shift from the line of free exciton in bulk crystal. We attribute the $B_1$-$B_5$ bands to some stable nanoclusters with size less than the size of zeolite Na-X supercage. We observed Stokes shift of the PL bands from the respective absorption bands. The nonmonotonic character of its dependence on the cluster size can be explained as the result of competition of the Frank-Condon shift and the shift due to electronic relaxation.

**S2Y139** **Doniach diagram and hydrogenation of the ternary compounds CePdX with X = In and Sn**

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Works devoted to the hydrogenation of intermetallics based on cerium, indicate that Hinsertion into the lattice induces generally an increase of the unit cell volume leading to a diminution of the coupling constant Jcf between 4f(Ce) and conduction electrons. A transition Kondo semiconductoranti-ferromagnet ferromagnet was evidenced by hydrogenation of CeNiSn [1]. We present the influence of hydrogenation on the structural and physical properties of the CePdIn and CePdSn. The former presents Kondo effect whereas the second exhibits a normal 4f(Ce) localized state. Their hydrogenation induces an increase of the Nel temperature (1.7 K3.4 K) for CePdIn and on the contrary, a decrease (7 K5.0 K) for CePdSn. These results compared to those obtained during the hydrogenation of CeNiIn (intermediate valenceferromagnet) and CeNiSn, can be explained on the basis of the Doniach diagram. [1] B. Chevalier et al., Chem. Mater. 15, 2181 (2003).

S2Y140 **Optical characterization of pristine and laser-treated nanostructured graphite films**

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Raman scattering is one of the most informative techniques for nanocarbon characterization. In this work a specific type of nanocarbon so called, coral -like graphite, has been studied. The films were deposited by CVD method. Afterwards the pristine material was treated with different trains of YAG:Nd laser pulses (1064 nm, 22 ns). The energy value per pulse reached 50 mJ. Raman spectroscopy has revealed a gradual changing of the film ordering depending on the laser fluence. The structure modification correlated with non-linear optical properties of the films. The work is supported by INTAS 01-254.

S2Y141 **Electrical Conductivity of Iron Oxide - Polypyrrole Nanocomposite**

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Nanocomposite of polypyrrole and iron oxide were prepared using simultaneous gelation and polymerization processes. Varied amounts of pyrrole were added to a solution containing an Fe(III) salt as precursor and 2-metoxy ethanol as solvent. The topology and the morphology of iron oxide nanoparticles in polypyrrole matrix were investigated in this paper by means of different investigation techniques (UV-Vis, X-ray diffraction and atomic force microscopy). AFM studies of powders deposited on glass indicated presence of nanosizes particles. Electrical conductivity studies of powders showed a slight variation in conductivity for lower concentration of pyrrole, with a sudden increase in conductivity at 15 percent of pyrrole concentration.

S2Y142 **Thermal Stability of Submicrocrystalline Structure of Metals Deformed by High-Pressure Torsion**

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Selected samples of Cu with addition of different amount of $Al_2O_3$, Fe, Mg and Mg with 10 wt. % Gd prepared by high-pressure torsion deformation under 6 GPa were studied by X-ray powder diffraction (XRD), positron life-time spectroscopy (PL) and transmission electron microscopy. XRD line broadening and total powder diffraction pattern fitting were used for crystallite size and dislocation density determination. PL spectra shown two major components from positrons trapped at dislocations and from positrons trapped in microvoids (4-5 vacancies). It was found that the addition of 0.5 wt. % $Al_2O_3$ prevents grain growth and keeps the dislocation density high up to about 400 C. However, above 300 C a few grains starts to grow rapidly, more in outer region of disc-shaped samples than in their center. Such inhomogeneity was not observed for Fe and Mg.

**S2Y143** **Anomalous Magnetic Anisotropy of Fe and Co Monatomic Wires at the Pt Surface Step Edge**

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We report a first-principles investigation of the anomalous magnetic anisotropy of quasi-one-dimensional ferromagnetic Fe and Co chains at the Pt(111) step edge. Our calculations for both Fe and Co wires show that magnetization is always confined in the plane perpendicular to the wire. The symmetry breaking at the step leads to an easy magnetization axis of Co wire at an odd angle of 20 towards the Pt step, in agreement with experiment. An effect becomes even stronger for Fe wire, with an easy magnetization axis at 30 towards the Pt step. Also, the Fe and Co spin and orbital moments become noncollinear, even in the case of a collinear ferromagnetic spin arrangement.

**S2Y144** **Reduction of Calcining Temperature in Preparation of YIG Powders Using High Energy Ball Milling**

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In this work mechanical alloying and subsequent heat treatment have been used to prepare ultrafine yttrium iron garnet (YIG) powders, using $FeCl_3$, $Y_2O_3$ and $Na_2CO_3$. The raw materials with appropriate ratio were loaded in a hardened steel vial in an Ar-filled glove-bag and milled in a Spex 8000D mixer/mill at different milling times. The influence of milling conditions and different heat treatments on phase formation and magnetic properties of the product were investigated. The structure was studied by x-ray diffraction and magnetic properties were measured on cold pressed isotropic cylindrical specimens, using a vibrating sample magnetometer (VSM). XRD studies show that a complete single phase of YIG was formed by subsequent heat treatment of the as-milled powder at 950 C, which is lower than the temperature associated with the conventional ceramic technique.

**S2Y145** **Förster energy transfer from a quantum well to a proximal nanocrystal-quantum-dot monolayer**

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We study theoretically and experimentally non-radiative Förster energy transfer from a quantum well (QW) to semiconductor nanocrystals assembled as a close-packed monolayer on top of the QW barrier. The calculated transfer rates are comparable to the rates of the radiative recombination of the QW excitations, indicating that the Förster transfer can be used as a mechanism for indirect electrical injection of charge carriers into the nanocrystals. Experimentally, we observe $\sim$50% transfer efficiencies that are limited by nonradiative carrier losses in the QW. We believe that nearly $\sim$100% efficiencies can be achieved by improving the QW quality and/or optimizing the geometry of the hybrid nanocrystal/QW structure.

S2Y146 **Dielectric Studies of Segmental Polyurethanes**

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We report our experimental results, on the electrical and dielectric properties of a set of novel polyurethanes and their dependence on the relative humidity. Broadband Dielectric Relaxation Spectroscopy(DRS) measurements were performed at several levels of water content (h). Special attention was paid to the conductivity effects (DC conductivity and Maxwell-Wagner-Sillars polarization).Thermally Stimulated Depolarization Currents (TSDC)have been employed for a more detailed study. The results show that the DC conductivity increases systematically with water content. For constant water content, DC conductivity depends sensitively on the morphology and the same is true, also for the characteristics of the MWS relaxation. Only at the highest values of h the details of the initial morphology become less important most likely due to the plasticization effect.

S2Y147 **AU CLUSTERS: THE ROLE OF ION ENERGY IN THEIR FORMATION**

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Clusters have been deposited by a monoenergetic mass selected ion beam with low energies (10-500 eV) on amorphous carbon substrates, which are used to minimize the influence of surface crystallography and ion induced structural changes. Gold clusters were deposited as a model system to study the ion energy dependence, the temporal evolution and the influence of the temperature on the cluster distribution. On the basis of the observations in Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) and X-Ray Photoelectron Spectroscopy (XPS), we demonstrate that the ion beam energy has a strong effect on the cluster size and we can easily control this parameter. In addition, nucleation and growth mechanisms of the gold clusters are discussed. Furthermore, the evolution of the clusters with temperature annealing has been studied in-situ by MXPS and TEM.

S2Y148 **Electronic switching and metal-insulator transitions in compounds of transition metals**

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Electrical instabilities of a kind (electroforming, threshold switching, memory effects) can be observed in a great variety of materials, particularly, in a number transition-metal compounds. There is a striking phenomenological similarity between switching and metal-insulator transition (MIT), and the switching effect has been treated in some works as a non-equilibrium phase transition occurring in electric field. In this communication, we report on various NDR (negative differential resistance) phenomena, both S- and N-type, in oxides of transition metals (V, Ti, Nb, Fe, W, Ta, Mo, Y, Mn, Hf, Zr), as well as in some other systems, including $V_2O_3$:Cr, Ni-S-Se, Cu-Ir-S-Se single crystals, and $V_2O_5$-gels. A universal switching mechanism is developed on the basis of the non-equilibrium electronically-driven MIT.

## S2Y149 INVESTIGATION OF THE VALENCE BAND ION THE CASE OF THIN FILMS OF RNi$_5$ (R=Ce,Y,La) COMPOUNDS

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The paper presents the evaluation by optical methods of the valence band shape in the case of inoxidized thin films of RNi$_5$ (R=Ce,Y, La) compounds. The results were correlated with those obtained by XPS spectroscopy for the same compounds yet not as thin films but bulk.

We used thin layers with insular (discontinuous) structure and thickness lower than 40 nm because of the presence of a number of surface states much higher than in the case of thin layers.

The determinations of the optical reflectance for the 1-10 eV domain lead to the determination of significant optical functions by the Kramers-Kronig formalism (n - index of refraction, k - absorption optical coefficient, $\epsilon_1$ - real part of dielectric permittivity, $\epsilon_2$ - imaginary part of dielectric permittivity).

The values of these functions for the domain studied show the properties of the distribution function of the state density in the valence band (VB) for energies higher than the Fermi energy.

The particularities of the $\epsilon_2$(h$\omega$) function are conditioned by the probability of optical transitions of the electrons on the free levels in the vicinity of the Fermi level EF and correspond to the maximums of the state density function. We noticed a good correlation with the results obtained by the XPS method for bulk compounds as well as the presence of specific energetic characteristic features.

## S2Y150 Piezoelectric anisotropy - phase transition relations in perovskite single crystals

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The orientation dependence of the longitudinal piezoelectric coefficient, $d_{33}^*$, is studied as a temperature function in $BaTiO_3$ and $PbTiO_3$ crystals using Landau-Ginzburg-Devonshire theory. We show that a presence of the ferroelectric-ferroelectric phase transitions in $BaTiO_3$ leads to enhanced $d_{33}^*$ along nonpolar directions. The reason for this is the abrupt increase of the shear piezoelectric coefficients in the vicinity of a phase transition temperature. In $PbTiO_3$, which does not exhibit FE-FE phase transitions, the shear piezoelectric effect is weak and $d_{33}^*$ has its maximum along the polar axis at all temperatures. These results can be generalized to include phase transitions induced by electric-field and composition variation and are valid for all perovskite materials, including complex relaxor-ferroelectric perovskites, with very large piezoelectric properties.

## S2Y151 Rapidly solidified Al-Cr-Fe-Si-Ti powder alloys - structure and properties

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Rapidly solidified RS aluminium alloys with transition elements form nanocrystalline and amorphous structures. These alloys show a high strength and good stability at elevated temperatures. Two powder Al-Cr-Fe-Si-Ti alloys, which differ in titanium content, were investigated. Microstructure and phase composition have been studied at elevated temperatures. Microstructure is formed of a(Al) matrix and uniformly dispersed intermetallic phases. Intermetallic phases Al13Cr2, Al82Fe18, Al84.6Cr15.4, Al80Cr20, Al95Fe4Cr and Al74Cr20Si6 were identified by X-ray diffraction. It was found, that alloy containing titanium showed a phase transformation between 400-500C (DTA). During long-term annealing a hardening due to decomposition of metastable phases and precipitation of intermetallic phases from supersaturated solution was detected.

S2Z201 **Poly(benzimidazole)/Layered Silicate Nanocomposites: Preparation, Silicate Exfoliation and Vapor-Barrier Properties**

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*3) Instituto de Fsica Gleb Wataghin, Universidade Estadual de Campinas*

Composites based on polybenzimidazole (PBI) and layered silicates: plain laponite (L), silylated laponite (SL) and functionalized montmorillonite MM (containg OH groups) were prepared by solution dispersion and casting. The following compositions (w/w) were prepared: PBI/L (90/10), PBI/SL (90/10), PBI/SL (80/20), PBI/SL (70/30), PBI/MM (90/10), PBI/MM (80/20), PBI/MM (70/30). X-Ray Diffraction (XRD) was used to investigate the possible exfoliation of the silicate platelets by PBI. Reflections related to the interlayer spacing of the silicates could be observed for all composites, except PBI/L (90/10) and PBI/SL (80/20). Moreover, the distance between the silicate platelets decreased after the compounding process, indicating that the water present in between the layers was removed during the casting process. The presence of the layered silicates caused a decrease in water and methanol permeability.

S2Z202 **Experimental studies of anomalous diffusion in membrane-gel system**

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We study one-dimensional diffusion in a membrane system including KCL gel solutions of different concentrations, separated by a horizontally located polymer membrane. We have filled the lower cuvette of the membrane system with an aqueous-gel KCl solution while the upper one - water gel. The diffusion can be characterized by a temporal evolution of the near-membrane layer (NML) thickness $\delta$. To observe the time evolution of NML we have employed the laser-interferometrical method. Recording the interferograms with a given time step, we have constructed the profile of KCl concentration. Our results of these studies allowed to determine that thickness of the NMLs in the studied membrane-gel system grows in time according to the relation $\delta(t) \sim t^{0.39}$ confirming a subdiffusive mechanism of KCl transport in the membrane system.

S2Z203 **MULTICOMPONENT CONFINED SYSTEM**

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We investigate critical behavior of finite-size multicomponent liquid system with geometry of a plane-parallel layer. For this system we find pair correlation functions of density fluctuations using iterational procedure. Namely, we get asymptotic solutions for pair correlation functions from Ornstain-Zernike (OZ) system of integral equations and then precise these expressions consequentially by using OZ systems of differential end integral equations. Basing on these results we analyze critical properties of the system. We show that when the system is at the close vicinity of critical hyper-surface in the space of thermodynamic variables it is possible to use only one correlation length to characterize its critical behavior. Moreover, in this case all the correlation functions are of the same structure so we propose some useful approximations that can be used when studying critical phenomena in such system. We also investigate influence of space limitations on the shift of critical parameters of the system and find that influence of boundary conditions on these shifts can be significant so in some cases it determines the sign of the effect. We analyze received results taking into account possibilities of their applying to experiments.

## S2Z204  Ordering at the interface of polymeric solutions

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Polymeric semiconductors, like substituted polythiophenes, are known to exhibit self-organisation into preferred crystalline orientation when deposited onto substrates. An understanding of the self-organisation is of pivotal importance for the successful exploitation of these semi-crystalline materials within molecular electronics and optronics. Employing in situ grazing incidence synchrotron x-ray diffraction we have found that the transformation from solution to solid phase often takes place within a skin on top of the polymer solution. The actual solidification process depends on the polymer concentration and the rate of blowing (of inert gas) above the solution surface. In fact, by controlling these two parameters the drying process may be tuned between two regimes: edge-drying and skin formation. The crystalline anisotropy in the resulting dry film depends on the choice of solvent.

## S2Z205  3D - structure of Emeraldine Base polymers by Car-Parrinello molecular dynamics.

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*3) NEST-INFM and Dipartimento di Fisica E. Fermi, Universita' di Pisa, Via Buonarroti 2, I-56127 Pisa, Italy*

We have studied the structural properties of the three dimensional crystalline regions of the EB-II polymers by means of first principle Car-Parrinello molecular dynamics. Using this technique we have provided the detailed morphology of each chain in terms of bond lengths, bond angles, torsion angles, and twisting and bending of the chain backbone. We have focused on the structural properties of the crystalline bulk of EB-II, analyzing, for the first time to our knowledge with this method, the effects on the single chains due to packing of the polymer chains which form the 3D crystal.
The simulation cell that we have used for the CP-MD calculations contains 8 strands of EB chains, each one with three phenilene rings, one quinoid ring, two amine (-N-) nitrogen atoms and two imine (-N=) nitrogen atoms, for a total of 192 carbon atoms, 32 nitrogen atoms, and 144 hydrogen atoms. The effect of environment on a single isolated chain has been clearly evidenced on a sound basis. In particular we have seen, for the first time, that the polymeric chains in the primitive cell are mutually shifted along the backbone axis by one complete ring; moreover it is evidenced the tendency of the backbone nitrogen atoms to be squeezed on a plane when inserted in a 3D structure, while ring-dihedral, ring-torsion and bond-angles within each chain are less sensitive to the presence of neighboring chains. On the optimal configuration found at T=0, we have calculated, together with the characteristic geometrical parameters of the structure, also the corresponding X-ray diffraction spectrum and pair correlation functions and have found good agreement with experimental measurements.

S2Z206 **Morphological Thermodynamics: how do free energies depend on shape?**

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We show that a thermodynamic potential of a fluid bounded by an arbitrarily shaped convex container can be calculated fully from the knowledge of only four morphometric measures. This remarkable result is based on the assumption that a thermodynamic potential is an "additive" functional which can be understood as a more precise definition for the conventional term "extensive". As a consequence, the surface tension and other thermodynamic quantities contain, beside a constant term, only contributions linear in the mean and Gaussian curvature of the container. Our findings are tested numerically in the purely entropic system of hard spheres bounded by a hard wall and substantiated by the behaviour of the density profile at the container wall.

S2Z207 **Composites and polymer mixtures super molecular structure study by very cold neutrons scattering.**

S. P. Kuznetsov[1],     N. P. Saposhnikov[1],     A. V. Shelagin[2],     P. N. Brevnov[3],     V. G. Grinev[3], N. Yu. Kovaleva[3], I. N. Meshkova[3], L. A. Novokshonova[3], T. M. Ushakova[3]
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*3) Semenov Chemical Physics Institute, Moscow, Russia*

Parameters of super molecular structure (SMS) of nano composie material montmorillonite/polyethylene obtained by polymerization filling method are determined by very cold neutrons scattering. Significant (three times) reduction of gas penetration for this material was found at achievement two per cents of montmorillonite nano particles volumeric share in a composite. It was found out that small additives of co-polymer polyethylene/polypropylene (PE/PP) clustered in amorphous layers of polimer mixture PP/(PE/PP). It was shown that crac temperature fall down with the increase of volumeric concentration of co-polymer particles in the mix.

S2Z208 **Casimir force between planar magnetodielectrics**

M. S. Tomaš[1]
*1) Rudjer Bošković Institute, Zagreb, Croatia*

Using the properties of the macroscopic field operators appropriate for absorbing magnetodielectric systems [H. T. Dung *et al*., e-print quant-ph/0306028] and deriving a convenient form of the relevant Green function for a multilayer, we calculate the Casimir force between two magnetodielectric stacks of layers. The resulting expression for the force, in terms of the reflection coefficients of the stacks, is of the same form as for a dielectric system [M. S. Tomaš, Phys. Rev. A **66**, 052103 (2002)], however, the Fresnel coefficients are modified because of the different magnetic properties of the system in the present case. We use this result to numerically explore the attractive/repulsive force between two thick (semi-infinite) magnetodielectric slabs described by the Drude-Lorentz type permittivities $\varepsilon_i(\omega)$ and permeabilities $\mu_i(\omega)$.

**S2Z209** **Monte Carlo Study of Hydrations Effects of Polar and Non-polar Molecules in Water at (250460)K.**

Atamas Nataliya[1], Atamas Alexander[1]
*1) Kiev Taras Shevchenko University*

In the present study includes results from Monte Carlo simulations study of hydrophobic hydrations of two-component systems water-polar or non-polar molecule (methanol and ethanol, dimethyl-ether and propane ) at range temperature from 250 to 460K. From radial distribution functions(RDF) the analysis of the local structure and energetic of solutions were done. The parameters of hydrogen bonds and the size of first and second hydrations shape ware determined. The influence of polar and non-polar solvent molecule on waters local structure, the hydrogen bonds nets and energetics ware analyzed. Radial distribution functions for water-water interactions calculated in pure water and water-dissolved molecule system are compared.

**S2Z210** **Self-Assembled Monodisperse Steroid Nanotubes in Water: Kinetics of Formation and Ordering**

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The kinetics of formation of lithocholate nanotubes was investigated. Small Angle X-Ray Scattering supported by Cryo-TEM pictures showed subtle structural variations. The interactions between the growing or reorganizing structures was probed by rheology. Stabilized highly monodisperse cylindrical tubes (outer diameter = 52 nm) with thin (1.5 nm) monomolecular walls are obtained through fast and complex morphological evolutions. The suspensions appear to be very shear-sensitive and are characterized by two temporal regimes. Upon increasing concentration or temperature the suspension undergo a transition towards a well-ordered hexagonal phase. This easy orientation of the nanotubes is a promising property for the design of bulk ordered and oriented materials.

**S2Z211** **Optical and refractometric studies of $(1-x)$TiO$_2 \cdot x$Ln$_2$O$_3$ (Ln= Nd, Sm, Gd, Er, Yb) thin films**

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$(1-x)$TiO$_2 \cdot x$Ln$_2$O$_3$ (Ln= Nd, Sm, Gd, Er, Yb; $x = 0.33, 0.5$) thin films, interesting for application in microelectronics, optics and medicine, were sputtered onto a quartz substrate. Ellipsometric and spectroscopic measurements have shown that with the increasing of molar mass due to the Nd $\rightarrow$ Sm $\rightarrow$ Yb substitution in the $0.67$TiO$_2 \cdot 0.33$Ln$_2$O$_3$ (Ln= Nd, Sm, Yb) system and to the Nd $\rightarrow$ Sm $\rightarrow$ Gd $\rightarrow$ Er substitution in the $0.5$TiO$_2 \cdot 0.5$Ln$_2$O$_3$ (Ln= Nd, Sm, Gd, Er) system a nonlinear increase of the film refractive index $n$ and nonlinear decrease of optical pseudogap value $\Delta E_g^*$ are observed. Contrary, a nonlinear decrease of the refractive index $n$ and nonlinear increase of optical pseudogap value $\Delta E_g^*$ are observed with the increase of Ln$_2$O$_3$ content.

S2Z212 **The influence of iron on electronic polarizibility in glasses of Sb-S-I type**

Imre O. Gúth[1], Željka N. Cvejić[1], Svetlana R. Lukić[1]
*1) Department of Physics, Faculty of Science, University of Novi Sad, 21000 Novi Sad, Trg Dositeja Obradovića 4, Serbia and Montenegro*

The oscillator force and resonance frequencies were determined for chalcogenide glasses of $Fe_x[(Sb_2S_3)_{0.75}(SbI_3)_{0.25}]_{100-x}$ system, where x=0, 0.1, 0.5, 0.8 and 1 at % of Fe. It is noticed that resonant frequency are practically independent on iron content in investigated glasses ($\omega_o$=9.07·$10^{14}$ Hz). The Sellmeir dispersion formula was used to describe the dispersion characteristics of the medium. We established analytic form of the oscillator force via iron content. The electronic polarizibility was also determined by using Lorentz-Lorentz relation. At given wavelength of incident light the electronic polarizibility decrease with increasing the density of glasses.

S2Z213 **Relaxation and dissipation processes in the phonon-impuriton system of superfluid mixture $^3$He in $^4$He**

V. Chagovets[1], T. Kalko[1], K. Nemchenko[2], E. Rudavskii[1], G. Sheshin[1], A. Zadorozhko[1]
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*2) V.Karazin National University, Kharkov, Ukraine*

The experimental data on effective thermal conductivity coefficient for superfluid mixtures $^3$He in $^4$He with the initial concentration of $^3$He 9.8% in the temperature range 70-500 mK has been obtained. New experimental data and earlier ones on effective thermal conductivity, shear viscosity, spin diffusion are adequately described within the framework of the phonon-impuriton kinetic theory of superfluid mixtures. The temperature and concentration dependenses for all times of relaxation processes are determined. It is found out the tree phonons processes bring the essential contribution to thermal equilibrium establishment even to concentrated superfluid mixtures. Phonon-impuriton relaxation times are calculated by phonon energy integration in limits where three phonon processes are allowed.

S2Z214 **Evolution of phonon pulses in superfluid $^4$He at different pressures**

I. N. Adamenko[1], K. E. Nemchenko[1], V. A. Slipko[1], A. F. G. Wyatt[2]
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*2) School of Physics, University of Exeter, Exeter EX4 4QL, United Kingdom*

We have considered the evolution of phonon pulses, propagating in superfluid $^4$He, at different pressures including two opposite cases: SVP and pressure above 19 bar. At relatively low pressures, when phonons interact strongly by three phonon (3PP) interaction, the system of equations for transverse evolution coincides with those for the system of gas-dynamics equations, describing the isothermal expansion of gas into vacuum. For longitudinal evolution we have derived the equation which has solution of a simple wave type. In the opposite limit case of high pressures above 19 bar, phonons do not interact by 3PP and propagate almost ballistically. Comparison between limiting cases has been made. It has been shown that in these two cases the region with initial energy density can exist rather long time in the centre of a pulse. For SVP and pressure 24 bar the comparison with the experimental data has been made.

**S2Z215** **Experimental Apparatus for Investigation of the Stability of the He II Flow Based on the Second Sound Attenuation Technique**

T.V. Chagovets[1], M. Rotter[1], F. Soukup[1], L. Skrbek[1]
*1) Joint Low Temperature Laboratory, Institute of Physics ASCR and Charles University*
*V Holesovickach 2, 180 00 Prague 8, Czech Republic*

An experimental apparatus for investigation of the stability of flow due to a torsionally oscillating cylinder in superfluid He II has been designed and constructed, based on the second sound attenuation for detecting quantized vortices in the flow. The probing second sound wave is generated and detected using the transducer /receiver gold-plated nuclepore membranes placed flush in the top and bottom plates of the resonator. Several second sound resonant modes can be used, by tuning the transducer frequency to a particular resonant mode. Computer-controlled stepper motor is used to set the oscillatory motion of the stainless steel cylinder 10 mm in dia, allowing for a broad range of dynamic parameter of the problem, the Taylor number. We discuss the preliminary results on the stability of the He II flow. This work is supported by the Czech Grant Agency No 202/02/0251.

**S2Z216** **Decay of Counterflow Turbulence in He II**

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*V Holesovickach 2, 180 00 Prague, Czech Republic*

We report investigation of the counterflow turbulence and its decay in three channels of different geometry based on the second sound attenuation technique. The counterflow turbulence is generated by applying the power to the heater placed in the closed end of the channel; when switched-off, the measured temperature difference across the channel quickly decays, in accord with the developed simple model. After the fast inital decay the second sound amplitude indicates a net increase of the observed vortex line density, which can be understood in terms of depolarization of the vortex tangle. After saturation time, the decay closely follows the classical -3/2 power law and for high enough initial vortex line density the decaying turbulence can be characterized by an effective kinematic viscosity. The influence of the channel geometry on the form of the observed deacy is discussed. This work is supported by the Czech Grant Agency No 202/02/0251.

**S2Z217** **SIMULTANEOUS SINGLET AND TRIPLET PAIRING IN A TWO-COMPONENT FERMI-LIQUID**

S. Shulga[1], A. Yatsenko[1]
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Coexistence of the Cooper pairs with different types of symmetry in a two-component Fermi-liquid is researched. The study is made using an example of the symmetrical nuclear matter with a nucleon Skyrme force. Our supposition is that the full spin of the pairs is equal to zero and isotopical spin takes values 0 and 1.

On the base of the Fermi-liquid approach (see, e.g. [1]) a system of the self-consistent gap equations is built and multi-gap solutions are obtained. Some thermodynamic properties of the solutions are examined.

1. A.I.Akhiezer et al., Physics Reports, 245, 1 (1994)

S2Z218 **Second Sound Turbulence in Superfluid Helium**

Maxim Yu. Brazhnikov[1], Viktor B. Efimov[1], German V. Kolmakov[1], Alexandr A. Levchenko[1], Elena V. Lebedeva[1], Leonid P. Mezhov-Deglin[1]
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Results of the new studies of nonlinear evolution of shape of the second sound waves in superfluid HeII in a resonator are presented. Analytical and numerical calculations shown that when the amplitude of periodical driving force has exceeded some critical value a power-like distibution of the amplitudes of waves over frequencies (the power spectrum) should be formed at frequencies higher than the driving frequency. This spectrum could be attributed to formation of the turbulent state. The range of frequencies, in which the power turbulent distribution is formed, is expanded toward high requencies as the amplitude of the driving force is increased. At high frequencies this range is limited by change of the mechanism of the energy transfer from nonlinear wave transformation to viscous damping. Change of the sign of the nonlinearity coefficient of second sound with lowering the temperature of HeII does not influence on shape of the spectrum.

S2Z219 **Instability of superfluid $^3$He-$^4$He solutions under heating from below**

V.K. Chagovets[1], T.V. Kalko[1], E.Ya. Rudavskii[1], G.A. Sheshin[1], A.A. Zadorozhko[1]
*1) B.Verkin Institute for Low Temperature Physics and Engineering, Kharkov, Ukraine*

The thermal instability of $^3$He-$^4$He mixture with the initial concentration of $^3$He 9.8% caused by heating the liquid from below has been studied experimentally. The temperature gradients in the mixture in the presence of different heat flows were measured. It is shown that the thermal convection develops at high temperature gradients. Thus the instability has been observed in a system with the light liquid at the top when there is no prerequisite for instability. In this case the Rayleigh numbers exceed many orders of magnitude those for heating from above. The results obtained are analyzed in terms of the theory of convective instability for binary mixtures. It is suggested that the phase separation of superfluid mixtures caused by a heat flow could be a destabilizing factor initiating instability. The vortex formation in superfluid helium and the related turbulent flows appearing at high temperature gradients can be another favourable factor for appearance of instability in liquid.

S2Z220 **Spherical electron systems in a multielectron bubble in liquid helium**

J. Tempere[1], I. F. Silvera[2], J. T. Devreese[1]
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*2) Lyman Laboratory of Physics, Harvard University, Cambridge MA, USA*

Multielectron bubbles are spherical cavities inside liquid helium, containing from a few up to $10^8$ electrons, that collect in a nanometer thin shell on the inner bubble surface, forming a spherical two-dimensional electron system. The spherical geometry influences the properties of the electron system with respect to a flat system. We discuss the formation of ripplonic polarons and show that using pressure to control the surface density of electrons, a quantum melting transition of the ripplopolaronic Wigner lattice should be accessible experimentally. The influence of a homogeneous magnetic field on the spherical electron gas is discussed and the occurrence of Landau bands in this system is shown.

S2Z221 **Tunneling Dynamics of a Superfluid Fermi Gas**

M. Wouters[1], J. Tempere[1], J. T. Devreese[1]
*1) TFVS, Universiteit Antwerpen, Universiteitsplein 1, B2610 Antwerpen, Belgium*

The search for Cooper pairing and superfluidity in a dilute gas of fermionic atoms has intensified as recent experiments have been able to form (bosonic) molecules from these fermionic atoms and Bose-Einstein condense these molecules. Superfluidity in a Cooper-paired Fermi gas may be revealed by the occurrence of Josephson currents in an optical lattice, since the observation of the Josephson effect constitutes an unambiguous proof of phase coherence accross different layers in the optical lattice. We derive, from a path-integral formalism, equations of motion for the density and the phase of the Fermi gas in an optical lattice. We find that in the BCS state, a dilute atomic Fermi gas will undergo Josephson oscillations in the lattice. These have recently been observed experimentally for bosons, and we predict the frequency at which they will occur for Cooper-paired fermions. We furthermore show that for superfluid fermions, tunneling between the layers of the optical trap is only suppressed in the strong-coupling (molecular) regime.

S2Z222 **Theory of Particle Image Velocimetry in helium II**

C.F. Barenghi[1], D.R. Poole[1], Y.A. Sergeev[2], W.F. Vinen[3]
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*2) School of Mechanical and Systems Engineering, University of Newcastle, UK*
*3) School of Physics and Astronomy, University of Birmingham, UK*

Recently two experimental groups have succedeed in implementing the classical Particle Image Velocimetry (PIV) method in liquid helium. The PIV method is based on injecting many small tracer particles in the liquid and detecting the velocity field at a given instant on a given plane by focusing into a narrow sheet two very short laser pulses separated in time by only few milliseconds. To interpret the PIV data correctly a key question must be answered: what do the tracer particles actually trace ? The question is far from trivial, given the two - fluids nature of helium II. In this work we present the governing equations of motion of the tracer particles and solve them in simple cases to capture the essential physics of the problem. We find that, depending on the parameters, in some situations the particles trace the normal fluid; in other, remarkably, they trace the superfluid.

# Plenary Session 8:30 – 9:00

P3A1    **Observation of the supersolid helium phase in solid He4**

Moses H.W. Chan[1]
*1) Pennsylvania State University, Pennsylvania, USA*

When liquid He-4 is cooled below 2.176K, it undergoes a phase transtion-Bose-Einstein condensation- and become a superfluid with zero viscosity. In 1995, Bose-Einstein condensation of alkali atoms in the vapor phase was achieved, adding to the list of superfluid system. Although it is counter to intuition, superfluid like behavior is thought possible even in solid helium. We have recently found evidence, through torsional oscillator measurements confirming the existence of the supersolid phase in solid helium confined in porous Vycor glass and also in bulk solid helium. These experiments were done in collaboration with Eunseong Kim and were supported by the National Science Foundation of the United States.

# Mini-Colloquia 9:15 – 11:15

*HTSC physics*　　　　　　　　　　　　　　　　　　　　　　　　　**Room B**

M3B1　**Are the spin-fluctuation and the electron-phonon mediated pairing potentials enhanced or suppressed by vertex corrections?**

W. Hanke[1]

*1) Theoretical Physics, University of Würzburg, D-97074 Würzburg, Germany*

The electron-phonon (el-ph) and the electron-spin-fluctuation (el-sp) vertices, which influence much-discussed issues such as the pairing potential and the "kinks" in ARPES spectra, are studied for the under-doped Hubbard model using numerically accurate Monte-Carlo (QMC) techniques complimented with diagrammatic approaches. Both el-ph and el-sp vertex corrections change even qualitatively when entering the physically relevant strong correlation regime ($U \cong 8t$): for the el-ph case forward (backward) scattering is significantly enhanced (suppressed) as a function of increasing U. This finding is not due to an incipient charge instability but due to a qualitatively different el-ph coupling in the strongly correlated (i. e. "spin bag") regime. The "spin bag" quasiparticle formation is also the reason behind the significant reduction due to vertex corrections of the effective el-sp interaction and the corresponding el-sp pairing potential found in our QMC studies.

M2B2　**Magnetic Excitations in High Temperature Superconductors**

Bernhard Keimer*[1]

*1) Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany*

We will present neutron scattering data on superconducting copper oxides with one, two, and three layers per unit cell, and we will argue that a universal picture of the spin dynamics in all of these materials is beginning to emerge. Proposals for the microscopic origin of this universal spin dynamics based Fermi liquid and striped states will be discussed in the light of recent data on the in-plane anisotropy of the spin dynamics in untwinned YBa2Cu3O6+x. In particular, we will show that stripe models are only compatible with these data if strong orientational fluctuations of the stripes are taken into account.

* Collaboration with V. Hinkov, C. Ulrich, S. Bayrakci, S. Pailhes, P. Bourges, Y. Sidis, A. Ivanov, A. Kulakov, C.T. Lin, D. Chen, and C. Bernhard

M2B3　**New Oxide-Superconductors: Similarity and Dissimilarity to High-Temperature Superconducting Cuprates**

Sadamichi Maekawa[1]

*1) Institute for Materials Research, Tohoku Univesrity, Sendai 980-8577, Japan*

Special attention has recently been paid to new oxide-superconductors on frustrated lattices. Cobalt-oxides (cobaltates) with triangular crystal structure and Os- and Re-oxides with pyrochlore structure show unique electronic and superconducting properties. The active electronic states are $t_{2g}$ with orbital degeneracy in these oxides in contrast with $e_g$ without degeneracy in high-temperature superconducting cuprates. Here, we present that the orbital degeneracy in $t_{2g}$ states on frustrated lattices brings the electronic structure which is different from the crystal structure [1,2]. A variety of the unique properties in the new oxide-superconductors are discussed in the light of the electronic states.

This work has been done in collaboration with W. Koshibae.

[1] W. Koshibae and S. Maekawa: Phys. Rev. Lett. **91**, 257003 (2003).
[2] W. Koshibae and S. Maekawa: Phys. Rev. Lett. **87**, 236603 (2001).

M2B4 **Quantum Magnetic Excitations from Stripes in Cuprate Superconductors**

J. M. Tranquada[1], H. Woo[1], T. G. Perring[2], H. Goka[3], G. D. Gu[1], G. Xu[1], M. Fujita[3], K. Yamada[3]

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We have used neutron scattering to investigate the magnetic excitations, up to 200 meV, in a stripe-ordered cuprate, $La_{1.875}Ba_{0.125}CuO_4$. We find that the excitation spectrum is quite similar to that found in recent studies of superconducting $YBa_2Cu_3O_{6+x}$, and that the measurements can be understood in terms of the quantum excitations of weakly-coupled antiferromagnetic spin ladders, where the ladders are defined by the charge stripes. JMT, HW, GDG, and GX are supported by the Office of Science, U.S. DOE under Contract No. DE-AC02-98CH10886.

M2B5 **How orderly is high Tc superconductivity?**

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Conventional superconductivity is well understood in terms of a theory resting on the understanding of the quantum gasses (Fermi- and Bose gas). In cuprate superconductivity a case has been developing over the years that the superconducting state is a highly organized entity which has little to do with a dilute gas of quantum particles. I will illustrate this 'fluctuating order' viewpoint using as an example a theoretical construct which is not necessarily of emperical relevance, but quite instructive regarding how far one can stretch the very notion of a quantum liquid. This is about a dislocation melted stripe phase, scrambling a spin-flux phase into an entity which is featureless except for its capacity to carry nodal fermions having the Senthil-Fisher topological interaction with the superconducting condensate.

*Physics of f-electron materials III. (PCFES 7)* **Room C**

M3C1 **Time-reversal-symmetry-broken superconductivity in the filled skutterudite PrOs$_4$Sb$_{12}$**

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The filled-skutterudite PrOs$_4$Sb$_{12}$ has been attracting much attention because of the fact this is the only Pr-based heavy-fermion superconductor [1]. Our muon spin relaxation measurements have revealed spontaneous appearance of static internal magnetic fields below $T_c$ [2]. This observation provides unambiguous evidence for "the breaking of time-reversal symmetry" in the superconducting state.
[1] E.D. Bauer *et al.*, Phys. Rev. B **65** (2002) 100506.
[2] Y. Aoki *et al.*, Phys. Rev. Lett. **91** (2003) 067003.

M3C2 **Unconventional Superconductivity and Magnetism in CePt$_3$Si**

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CePt$_3$Si is a novel non-centrosymmetric heavy fermion superconductor which orders antiferromagnetically below 2.2 K and enters into a superconducting ground state at 0.75 K. The most striking features are: superconductivity coexists with long range antiferromagnetic order on, most likely, different regions of the Fermi surface. We show how superconductivity and long range magnetic order develops upon doping.

M3C3 **Coexistence of ferromagnetism and superconductivity in the strongly correlated transition metal compound ZrZn$_2$**

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The recent observation of the coexistence of ferromagnetism and superconductivity in ZrZn$_2$ has brought a revival of interest in this material. In the beginning of the 80s, it had been conjectured that the longitudinal spin-fluctuations could lead to spin-triplet *p*-wave superconductivity. I will present here the results from our *ab-initio* electronic structure calculations using the LMTO method within the local spin density approximation, as well as the excellent agreement between those and several recent experimental results. From our electronic structure, we calculated the generalised susceptibilities in order to investigate the viability of longitudinal spin-fluctuation-induced spin-triplet *p*-wave superconductivity in the ferromagnetic state. We found a critical temperature, $T_c$, of the order of 1 K and that the spin fluctuations prevent the onset of conventional *s*-wave superconductivity in spite of the presence of strong electron-phonon coupling.

M3C4 **Pressure-Induced Superconductor-Insulator Transition in Chalcogenide Spinel Compounds**

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We carried out resistivity $\rho$ measurements in chalcogenide spinels under pressure using a cubic-anvil device, and found a pressure-induced superconductor-insulator (SI) transition at a critical pressure $P_{SI}$ between 5.0 and 5.6 GPa in $CuRh_2S_4$. This compound is a metal above $T_c$ = 4.7 K under the ambient pressure. It is remarkable that $\rho$ at 10 K is enormously enhanced by over 7 orders of magnitude with increasing $P$ up to 8.0 GPa. The resistivity shows no metallic temperature $T$ dependence above $P_{SI}$ in the whole $T$ range measured. A mechanism of the metal-insulator (MI) change in the transport property in the normal state is a key to understand the SI transition. We present candidates for the origin of the MI transition in conjunction with transport properties of other chalcogenide spinels.

*Magnetic quantum phase transitions and related phenomena* **Room D**

### M3D1 Nexus Between Quantum Criticality and Phase Formation: The Case of URh2Si2

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Quantum criticality is becoming increasingly recognized as a controlling factor in the creation of novel phases, e.g. unconventional superconductivity. However, direct proof for a causal link between the quantum fluctuations and the phase formation remains a formidable experimental challenge. URu2Si2 is an example of a strongly correlated electron system where signatures of quantum criticality appear at very strong magnetic fields indicating the existence of a quantum critical point (QCP) hidden beneath a complex region of interconnecting phases. Using a variety of thermodynamic and transport measurements we map out the field/temperature phase diagram and establish the QCP at 37 T. We then show how Rh doping simplifies the phase diagram eliminating all but one of the phases while preserving the robust QCP.

### M3D2 Magnetic Correlations near Quantum Critical Transitions

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We have used neutron scattering measurements to explore the development of spatial and temporal correlations in the vicinity of magnetic quantum phase transitions. We compare here two systems, one with an antiferromagnetic quantum critical point $Ce(Ru_{1-x}Fe)x)_2Ge_2$ ($x_C$=0.76), and the second $Zr_{1-x}Nb_xZn_2$ ($x_C$=0.05) with a ferromagnetic quantum critical point. In the first system, the zero temperature divergence of the susceptibility is controlled by extended fluctuations, leading to non-Fermi liquid energy/temperature scaling, absent in paramagnetic $Ce(Ru_{1-x}Fe_x)_2Ge_2$ ($x$=0.85). We have performed small angle neutron scattering (SANS) measurements on the itinerant ferromagnet $ZrZn_2$ and on quantum critical $Zr_{1-x}Nb_xZn_2$ ($x$=$x_C$=0.05). In $ZrZn_2$, magnetic correlations are present at temperatures as large as 3 $T_C$, although the approach to magnetic order in quantum critical $Zr_{1-x}Nb_xZn_2$ ($x$=$x_C$=0.05) is much more abrupt, with a substantial compression of the scattering to smaller wave vectors at low temperature.

### M3D4 Ferromagnetic quantum phase transitions

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We discuss the theory of ferromagnetic quantum phase transitions in metals. These transitions are prime examples of a paradigm that has become of increasing importance in the theory of quantum phase transitions, namely, the coupling of the order parameter fluctuations to other soft modes. These other soft modes are manifestations of generic scale invariance, i.e., the appearance of long-range correlations in whole regions of the phase diagram. In clean metals, these mode-coupling effects generically lead to a fluctuation-induced first-order transition. In disordered metals, the transition is of second order, but with unusual non-mean-field critical exponents. We also discuss recent developments concerning the importance of rare regions on the transition in disordered metals: For Ising order parameter symmetry, rare region effects can become so strong that they destroy the sharp transition by smearing.

M3D5 **Topological excitations and fractionalization at quantum phase transitions**

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The theory of second order phase transitions is one of the foundations of modern statistical mechanics and condensed matter theory. A central concept is the observable 'order parameter', whose non-zero average value characterizes one or more phases and usually breaks a symmetry of the Hamiltonian. At large distances and long times, fluctuations of the order parameter(s) are described by a continuum field theory, and these dominate the physics near such phase transitions. In this talk I show that near second order quantum phase transitions, subtle quantum interference effects can invalidate this paradigm. I present a theory of quantum critical points in a variety of experimentally relevant two-dimensional antiferromagnets. The critical points separate phases characterized by conventional 'confining' order parameters. Nevertheless, the critical theory contains a new emergent gauge field, and 'deconfined' degrees of freedom associated with fractionalization of the order parameters. Applications of these ideas to critical heavy electron metals will be discussed.

*Fluid interfaces* **Room E**

### M3E1   Ions at the air/water interface

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There is increasing evidence that the air/water interface is of a key importance in many chemical processes in the atmosphere, such as the release of reactive halogen species from aqeous sea salt aerosols in the marine boundary layer or tropospheric ozone destruction in the Arctic during polar sunrise. Despite this, little has been known about the structure and physical properties of aqueous aerosols at a detailed, molecular level. Here, we summarize results of classical molecular dynamics, Car-Parrinello molecular dynamics, and ab initio quantum chemistry calculations on concentrated aqueous salt solutions confined to cluster and slab geometries. The main questions addressed by the simulations concern the distribution of ions at the surface and in the aqueous bulk, the onset of ionic solvation in water clusters, transition from clusters to slabs, and structure of solvation layers. A key result of the simulations is the observation that polarizable anions (e.g., chloride, bromide, and iodide) are present at the air-water interface of bulk solutions in amounts sufficient for the heterogenous atmospheric chemistry to take place. The calculations also reveal that bromide and iodide actually exhibits surfactant activity, i.e., their concentration at certain regions of the interface is higher than in the bulk. This is in direct contradiction with the standard Onsager model of the surface of electrolytes, however, it is an accord with the observed atmospheric reactivity of aqueous bromide and chloride, and with recent spectroscopic and SEM experiments.

### M3E2   Microscopic structure of fluid interfaces

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Molecular orientations at surfaces play a key role in many interesting optical properties of thin films and interfaces. Accurate determination of 'molecular tilt' angles and their distribution is therefore essential for interpreting measurements at interfaces such as X-ray scattering experiments and spectroscopic techniques. In particular the nanoscopic structure of binary liquid interfaces is still poorly understood because fluctuations of the composition occur in addition to capillary waves. Starting from a microscopic density functional theory for inhomogeneous fluids we derive an effective interface Hamiltonian which goes beyond the common phenomenological capillary-wave description. Explicit expressions are given for the surface energy, the bending rigidities and especially the couplings of compositional waves as well as for the distribution of local interface orientations. Comparision of the theoretical predictions with synchrotron scattering experiments allow a quantitative determination of microscopic interaction parameters of the fluid.

### M3E3   Surface energy of liquid interfaces: an x ray synchrotron study

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Liquid-vapour interfaces were first described by van der Waals in 1894 as regions of continuous variation of density. In contrast the 1965 capillary-wave model assumes a step like local density profile across the interface whose width is the result of the propagation of thermally excited capillary waves. This model has been validated for length scales of tenths of micrometres and larger and is expected to break down on smaller length scales. We have investigated the submicrometre structure of these interfaces using x ray scattering. We find that the effective momentum-dependent surface energy first decreases from its macroscopic value and then increases with increasing wave vector, in quantitave agreement with a recent density functional theory. We then turned to surfactant monolayers at the water-air interface: x ray scattering gives access to the bending energy of the films. The underlying molecular mechanisms can be discussed using different models.

M3E4 **Bending self-assembled amphiphilic monolayers**

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The phase behaviour of microemulsions and the coalescence process in macroemulsions depend on the elastic properties of the interface, e.g. the interfacial tension and bending rigidity. These properties depend in turn on the presence of surfactants - amphiphilic molecules that self assemble on the oil/water interface in many natural and industrial emulsions. We used a mesoscopic oil/water/surfactant model and large-scale Dissipative Particle Dynamics simulations to find out how the surfactants' structure affects the elastic properties of these monolayers[1]. We confirmed the mean-field theory prediction that the monolayer bending rigidity obeys a power-law increase with chain length. However, the actual exponent is lower, due to lower surface densities for longer chains. In the lecture we will discuss the connection between surfactant structure, monolayer rigidity, and film rupture. (1) L. Rekvig, B. Hafskjold, and B. Smit, Phys. Rev. Lett. 92, 116101 (2004)

*Carbon nano-tubes* **Room F**

M3F1 **Phonons in carbon nanotubes**

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Phonon dispersions for single- and double-wall carbon nanotubes (SWNT and DWNT) are found. For SWNTs the dynamical model is based on the kinematically and dynamically adjusted (for each nanotube) force constants. It is also used for the intra-wall interaction in DWNTs, with the inter-wall Lenard-Jones or Kolmogorov-Crespi potential. Calculations include full symmetry of the tubes (code POLSym implementing modified group projector technique), enabling large scale analysis of various characteristics. Particularly, for more than 1000 SWNTs frequency/diameter-chirality dependance of all Raman and infra-red active modes is given. For DWNTs the numerical results are interpreted within simple coupled oscillator model. Besides breathing like and high-energy modes, the low frequency rigid layer modes are analyzed in the context of low inter-wall interaction and possible super-slippery modes as a consequence of the symmetry breaking. [1] M.Damnjanovic et al., Phys. Rev. B 69 (2004) 153401-1-4

M3F2 **Curvature effects in the electronic properties of small diameter single-walled carbon nanotubes**

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First principles calculations will be presented on the optimized geometry and the band structure of 40 different single-walled carbon nanotubes with small diameter, including 14 chiral tubes. Density functional theory is employed in the calculations. The band gaps of the semiconducting tubes as well as the position of the Fermi wave vector of the armchair tubes are calculated and discussed.

M3F3 **Resonant character of Raman scattering in single-wall carbon nanotubes confirmed by photoluminescence measurements**

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Aqueous suspensions of individual single-wall carbon nanotubes (SWNT) provide a unique possibility to observe simultaneously photoluminescence (PL) and Raman spectra for semiconducting SWNT. An excitation energy variation leads to changing of relative spectral position of PL and Raman bands. They overlap when the resonant Raman process takes place for outcoming photons. This allows to estimate the enhancement "windows" for one- and two-phonon Raman bands. In this work the Raman and PL spectra have been measured for arc and HiPCO SWNT. Ti:sapphire laser (700-1000 nm) was used for excitation. The experimental data on resonance "windows" have been compared with the predicted values of $E_{11}$ optical transitions for different tubes. Thanks to RFBR 04-17618.

M3F4 **LOW-ENERGY ELECTRONIC STRUCTURE OF INTERCALATED SINGLE WALL CARBON NANOTUBES**

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In this contribution we report on a direct observation of a transition from a Tomonaga-Luttinger liquid to a Fermi liquid behavior in potassium intercalated mats of single wall carbon nanotubes (SWCNT) using high resolution photoemission spectroscopy as probe. An analysis of the spectral shape near the Fermi level reveals a Tomonaga-Luttinger liquid power law scaling in the density of states for the pristine sample and for low dopant concentration. As soon as the doping is high enough to fill bands of the semiconducting tubes a distinct transition to a bundle of only metallic SWCNT with a scaling behavior of a normal Fermi liquid occurs.

M3F5 **C60 excitations in Peapods : an inelastic neutron scattering investigation**

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In this communication, I discuss recent results obtained on $C_{60}$ confined into SWNT (peapods). Much attention will be done on the low-frequency part of the vibration spectrum. Unique information on the low-frequency excitations is derived from the vibrational density-of states (DOS) measured by inelastic neutron scattering (INS) experiments.
The density-of-states of peapods organized in bundles has been measured in the 100 K-480 K temperature range. The low-frequency DOS of $C_{60}$ confined into SWNT displays well defined features around 2 meV and 5 meV assigned to libration and interball translation modes. Additional contributions between 8 and 20 meV questions the organisation of $C_{60}$ molecules inside the tubes: $C_{60}$ linked by van der Waals interaction, polymerized $C_{60}$ inside the tubes, confinement effect on the vibrations of the $C_{60}$ molecules?

M3F6 **(*n,m*) Chirality Assignment Based on Resonant Raman Scattering**

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Resonant Raman scattering is a well-known method for the investigation of optical transitions in solids. Here we show that by studying the radial breathing mode, we can derive an assignment of the chiral indices of carbon nanotubes. Different from luminescence measurements, the chirality of both semiconducting and metallic nanotubes can be investigated. Our assignment is based on a plot of the resonance maxima of the radial breathing modes *versus* inverse RBM frequency. These maxima shift through the spectra in *laola*-like waves and are compared to third-nearest neighbor tight-binding energies in a so-called Kataura plot. From a comparison of $\approx 40$ different-chirality nanotubes we find independent of any prior assumptions $\omega_{RBM} = (216 \pm 2)\,\mathrm{cm}^{-1}\,\mathrm{nm}/d + (17 \pm 2)\,\mathrm{cm}^{-1}$.

*Molecular dynamics studies of surfaces processes* **Room G**

M3G2 **Simulation of surface diffusion**

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The study of surface diffusion is a key step in understanding many surface phenomena, such as surface reactions and epitaxial crystal growth. In particular, the knowledge of the elementary diffusion mechanisms allows to build up reliable models helping the interpretation of crystal growth experiments. With this respect, the interplay between experiments and simulations is crucial. Here we briefly overview the different simulation methods which are used in the modelling of surface diffusion processes. These range from Langevin simulations, to Molecular Dynamics and to accelerated Molecular Dynamics. As specific examples, we focus on Molecular Dynamics simulations of the diffusion of adatoms and small clusters on anisotropic metallic surfaces, and on Langevin simulations of systems where diffusion proceeds by long jumps.

M3G3 **Submonolayer growth with impurities: Attractive vs. repulsive impurity-adatom interaction.**

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The submonolayer regime of homoepitaxy is broadly used in microscopic studies of the surface diffusion. The presence even of a small amount of impurities can have dramatic effects. Influences of impurities on growth mechanism depending on impurity characteristics (mobility, type and strength of interaction) are evaluated using KMC simulations and rate equations. It is demonstrated that attractive immobile impurities can cause an order of magnitude increase of island density. Comparison of growth scenario for attractive and repulsive impurities shows that the dependence of saturated island density on the impurity concentration is an important quantity for the assessment of interaction type. In particular, we present results for effect of oxygen on Al epitaxy. Consequences of the effects caused by impurities for the analysis of STM measurements of the diffusion coefficient are discussed.

M3G4 **Decay mechanisms of nanoislands Monte Carlo simulations**

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Classical thermodynamic theories which are based on the Gibbs Thomson relation have been used to describe the decay of nanoislands under steady state conditions. With Monte Carlo simulations we show that for islands of sufficiently small radius such average thermodynamic description does not apply. The shape of vacancy and adatom islands as well as decay of islands depends on the energy barriers of individual detachment processes. The microscopic structure at the island edge becomes the key controlling process. This leads to a different dependence of the average detachment rate and different decay law than the one deduced from the thermodynamic theory. This analysis is applied on Ag(111) for the standard geometry of adatom and vacancy island decay within a larger vacancy island; to deduce the controlling microscopic barriers and the interlayer probability. We discuss the possibility to deduce Ehrlich-Schwbel barrier from the decay experiments.

M3G5 **Surface friction, lubrication, and atomistic simulation**

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Of the three main contributions to sliding friction, namely non-abrasive mechanical dissipation, abrasive mechanical dissipation (wear), and electronic dissipation (for metals), molecular dynamics atomistic simulation is best at describing basically the first. After a brief introduction to non-abrasive sliding friction between atomically flat surfaces (the pinned regime of a lubricant, the stick-slip motion, the superlubricity regime) I will outline molecular dynamics simulations of two prototype problems. They are the sliding of a solid molecular layer on a metal surface, e.g., in quartz microbalance experiments, and the squeeze-out of a thin fluid lubricant film clamped between two solid surfaces, a central problem of boundary lubrication. Detailed results will be presented for the latter, clarifying the main role of adhesion versus viscosity.

*Nitrogen bonds and bands in diluted nitrides* **Room H**

**M3H1** **Theory of the electronic structure of dilute nitride alloys: beyond the band-anti-crossing model**

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The band anti-crossing (BAC) model describes well the strong band-gap bowing observed in $GaN_xAs_{1-x}$ and related alloys. Despite its successes, the BAC model remains controversial. It omits much detail of the band structure, including in particular the effects of the inevitable random disorder present in such alloys. Detailed studies show a range of resonant defect levels close to the conduction band (CB) edge. How do these influence the BAC model and its predictions? We show, using the tight-binding method, that a quantitative description of the CB away from the zone centre requires to combine the BAC model with more detailed calculations of nitrogen cluster states. These quantiatively explain the anomalously large electron effective mass observed in $GaN_xAs_{1-x}$ samples, and also place a fundamental limit on the electron mobility in this novel alloy system.

**M3H2** **Probing the electronic properties of dilute nitrides by carrier localization and effective mass measurements**

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We studied the electronic properties of InGaAsN alloys by magnetophotoluminescence (m-PL) in a wide range of N concentration between 0 and 5%. The electron effective mass and exciton radius undergo a sudden increase and decrease, respectively, in a very narrow interval of N concentration centred at y=0.1%. Alloying of GaAsN with In (30%) results in a shift of such interval to y=1.0%. These findings provide firm guidelines to models aimed at describing the electronic properties of dilute nitrides. Also, m-PL shows that the origin of the radiative recombination at low temperature (T<100 K) is not excitonic, and is due to free holes recombining with electrons localized in N-rich regions.

**M3H3** **Band structure and laser characteristics of the Ga(In)NAs/GaAs QWs: comparison of the theory with experiment**

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We derive an analytical model to describe the conduction band states of GaNAs-based quantum well structures [1], including the band anti-crossing (BAC) effect between N resonant states and the conduction band edge. The predictions of the model are compared to those obtained using a full 10-band $\mathbf{k} \cdot \mathbf{p}$ model based on the same set of parameters [2]. Both methods are then tested by comparison with the experimentally determined ground and excited state interband transition energies of $GaN_xAs_{1-x}$ quantum wells of different well widths and N composition, $x$, obtained at 300 K and under hydrostatic pressures up to 2.0 GPa [3]. We show that the transition energies can be described by a consistent set of material parameters in all the samples studied, and present how the conduction to valence band offset ratio varies strongly with $x$ in $GaN_xAs_{1-x}$/GaAs quantum well structures. We conclude that the model presented can be used to predict the transition energies and electron subband structure of any $GaN_xAs_{1-x}$/GaAs quantum well with well width between 2 and 25 nm, and N composition $x$ between 1 and 4%, although further work is still required to confirm the optimum choice for the variation of band offset ratio with composition. After introducing the 10 band $\mathbf{k} \cdot \mathbf{p}$ Hamiltonian, we present a comprehensive theoretical and experimental analysis of 1.3 $\mu$m GaInNAs/GaAs lasers [2]. Our calculations show that the addition of N reduces the peak gain and differential gain at fixed carrier density, although the gain saturation value and the peak gain as a function of radiative current density are largely unchanged due to the incorporation of N. The gain characteristics are optimized by including the minimum amount of nitrogen necessary to prevent strain relaxation at the given well thickness [4]. The measured spontaneous emission and gain characteristics of real devices are well described by the theoretical model. Our analysis shows that the threshold current is dominated by non-radiative, defect-related recombination. Elimination of these losses would enable laser characteristics comparable with the best InGaAsP/InP-based lasers with the added advantages provided by the GaAs system that are important for vertical integration.

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**M3H4** **Growth and Structural Characterization of (GaIn)(NAs)**

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*Superconducting qubits* **Hall J**

M3J1 **Experimental Studies of a Josephson Charge Qubit with RF-SET read-out**

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In order to experimentally realize a superconducting charge qubit, one must overcome several challenging problems. The first, which is surprisingly subtle and difficult, involves producing Cooper-pair-boxes with robust even-parity states. One must then optimize the readout while simultaneously minimizing its back-action on the qubit. Finally, the mechanisms of decoherence in Josephson junction qubits must be understood if we are to scale up to many qubits. We must identify both the sources of dephasing and relaxation, and how they couple to the qubit. Although there is much to learn from the mature field of spin physics, superconducting qubits are fundamentally different in that they are mesoscopic objects, the noise is very asymmetric, and readout involves measurements of a single system as opposed to an ensemble.

We present experimental studies of a Josephson charge qubit (Cooper-pair-box) that uses radio-frequency, single-electron-transistor (RF-SET) readout. We describe the evolution of our sample fabrication process that led to robust even-parity boxes with SET's that can be operated in the sub-gap regime in a manner that minimizes the backaction. Fast DC pulses are used to manipulate the qubit and coherent oscillations with a high fidelity are consistently observed. The reduction from 100pulse rise-time. Measurements of dephasing for the full range of gate charge and on time scales extending to the sub-nanosecond regime have been made. These allow us to attribute the main source of dephasing to fluctuations that couple predominantly to charge.

M3J2 **Tansfer of quantum information through Josephson arrays**

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Josephson junction arrays can behave as a quantum channels and used to transfer quantum information between distant sites. In this work we discuss simple protocols to realize, withouth external control, state transfer with high fidelity in Josephson chains. The great advantage of these schemes is that they not require complicate gating but use the natural dynamics of a properly designed array. We propose an experiment, realizable with present-day technology, that may allow to implement these protocols. We calculate the fidelity of the channel and also analyze the readout process of the transferred state at the end of the array. Finally, we show that transmission through the array is relatively robust with respect to disorder and other experimental imperfections.

M3J3 **Telegraph and $1/f$ noise in Josephson qubits: decoherence and quantum control**

E. Paladino[1], A. D'Arrigo[1], A. Mastellone[1], G. Falci[1]
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We study decoherence in Josephson qubits due to bistable quantum fluctuators [1] modeling fluctuating impurities responsible for $1/f$ charge noise, and discuss quantum control protocols [2]. We investigate various computation procedures (single shot measurements, repeated measurements, echo protocols) at different working points. Our results qualitatively explain recent observations of splittings of spectroscopic peaks, inhomogeneous broadening, beats and dead zones in the dynamics. Dynamical decoupling protocols compensate or enhance the noise, depending on the nature of the impurities, on the pulse frequency and on the operating point. Results are interpreted in terms of quantum Zeno and inverse Zeno effect. The rich physics emerging suggests that decoupling techniques may be employed for spectroscopy of the environment.

[1] E. Paladino, et. al. PRL, 88, 228304,(2002). [2] G. Falci, et. al., cond-mat/0312442.

M3J4 **Charge and flux controlled pumping of Cooper pairs**

J. P. Pekola[1], A. O. Niskanen[2], J. M. Kivioja[1], H. Seppä[2]

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We discuss adiabatic transport of Cooper pairs in Josephson junction based pumps. As a specific example, we discuss the principle, theory and the first experimental results on a Cooper pair "sluice", where charge is controlled by both magnetic flux and gate voltage. This device shares many features with Josephson jumction based quantum bits. Influence of non-adiabaticity and phase fluctuations on the operation of charge pumps will be described.

M3J5 **Adiabatic passage in superconducting nanocircuits**

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With the rapid technological progress in quantum-state engineering in superconducting devices there is an increasing demand for techniques of quantum control. Stimulated Raman adiabatic passage (STIRAP) is a powerful method in quantum optics which has remained largely unknown to solid-state physicists. It is used to achieve highly efficient and controlled population transfer in (discrete) multilevel quantum systems.

Apart from other potential applications in solid-state physics, adiabatic passage offers interesting possibilities to manipulate qubit circuits. In this presentation, we explain the idea of the method and describe examples of controlled quantum dynamics in superconducting nanocircuits by applying adiabatic passage.

M3J6 **Entanglement spectroscopy of a driven solid-state qubit and its detector**

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*3) Institut für Theoretische Physik, Universität Regensburg, 93035 Regensburg, Germany*

We study the asymptotic dynamics of a driven quantum two level system coupled via a quantum detector to the environment. We find multi-photon resonances which are due to the entanglement of the qubit and the detector. Different regimes are studied by employing a perturbative Floquet-Born-Markov approach for the qubit+detector system, as well as non-perturbative real-time path integral schemes for the driven spin-boson system. We find analytical results for the resonances which agree well with those of ab-initio calculations. For some cases a complete inversion of population is found.

# Poster Session 11:15 – 12:30

**S3X1** **Reflection of surface spin waves from semi-infinite uniaxial multilayer ferromagnetic structure**

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Reflection of spin waves is investigated on the boundary of homogeneous and multilayer ferromagnetic media. The external homogeneous magnetic field and easy axis of homogeneous and multilayer parts are parallel to the plane of contact of layers. Multilayer part consists of alternating layers with different parameters of uniaxial anisotropy, exchange interaction and saturation magnetization. Exchange interaction in interfaces is taken into account by $\delta$-function-like item in the energy. The dependencies of reflection coefficient on frequency and magnetic field are obtained. They show an opportunity to operate the reflectance by changing the value of magnetic field for chosen frequency at fixed parameters of the system. The influence of the properties of interface expressed by interlayer exchange parameter is also explored. It is shown, that in the diapason of small values of this parameter the character of spin wave reflection changes especially essentially.

**S3X2** **Incommensurate magnetic structure in the spin-chain cuprate LiCu2O2 as seen by NMR**

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*2) Ural State University, 620083, Ekaterinburg, Russia*
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6,7Li NMR measurements of the spin-chain compound LiCu2O2 in the paramagnetic and magnetically ordered states are presented. Below T=24 K the NMR lineshape presents a signature of incommensurate (IC) spiral modulation of the Cu magnetic moments. 7Li NMR reveals strong phason-like dynamical fluctuations below 24 K. The intrinsic incommensurability is believed to be responsible for an unconventional evolution spin structure with a series of phase transitions (24.2, 22.5 and 9 K). We elucidated a strong in-chain frustration and also the microscopic origin of the magnetic spiral.

**S3X3** **Resonance heat transport between two solids through multiplayer interface**

A. Feher[1], A. Ya. Dulfan[2], P. A. Minaev[3], A. G. Shkorbatov[3], E. S. Syrkin[3]
*1) Safarik University, Department of Experimental Physics, Kosice, Slovakia*
*2) Physics technology dept., National State University KPI, Kharkov, Ukraine*
*3) Institute for Low Temperature Physics and Engineering NASU, Kharkov, Ukraine*

Experimentally observed solid-solid thermal resistance shows essential features. The mechanism of the resonance transport of phonons considered in the present work is characteristic for heat transmission between two media. In point contacts molecules of water or solidified inert gases can serve as a resonance layer. Peaks of the reduced heat flow considered in the present work are observed, for example, in KBr-KBr, KBr-Cu. In these contacts a low-temperature maximum observed can be explained by the theory of the resonance transport. Multichannel resonance transmission of phonons through the interface of the point contact Si-Cu was studied using the capillary effects theory. The results obtained are in a good agreement with the experimental data.

**S3X4** **Electron coherent dynamics after intersubband excitation**

Antonio Hernandez-Cabrera[1], Pilar Aceituno[1], Fedir T. Vasko[2]
*1) Dpto. Fisica Basica. Universidad de La Laguna. La Laguna 38206-Tenerife. Spain.*
*2) Institute of Semiconductors Physics. NAS of Ukraine. Kiev, 252650. Ukraine.*

We study the temporal behaviour of the dipole moment and the photoinduced concentration of electrons in tunnel-coupled quantum wells after an ultrafast intersubband photoexcitation. We take into account dephasing and population relaxation processes to analyse the nonlinear regime of the response. We also include the dependencies on the structure parameters, the detuning frequency and the pump duration. The coherent dynamics of electrons is studied within the framework of the matrix density formalism. Results show different behaviours for transitions from a single ground level to coupled excited states and transitions from coupled states to a single excited state.

**S3X5** **Optical properties of indirect excitons in in-plane magnetic fields**

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*1) Institute of Physics, Charles University, Praha, Czech Republic*
*2) Grenoble High Magnetic Field Laboratory, CNRS, Grenoble, France*
*3) Institut für Technische Physik I, University Erlangen, Germany*

High magnetic field photoluminescence (PL) measurements of a GaAlAs/GaAs double quantum well are reported. The properties of spatially indirect excitons (IX), i.e. electron-hole pairs where particles are localized in opposite quantum wells, are studied. We show that in contrast to the previously published strong PL intensity quenching in high in-plane magnetic field [1,2], which was successfully explained by the particle in-plane momentum conservation, the IX PL survives up to the magnetic field of 22 T in our structures. We relate our observation to the IX localization and consequently to their enhanced radiative recombination.
[1] A. Parlangeli et al., Phys. Rev. B 62, 15 323 (2000)
[2] L. V. Butov et al., Phys. Rev. B 62, 1548 (2000)

**S3X6** **Trion dynamics in asymmetric coupled quantum wells**

Pilar Aceituno[1], Antonio Hernandez-Cabrera[1], [1]
*1) Dpto. Fisica Basica. Universidad de La Laguna. La Laguna. 38206-Tenerife. Spain*

The coherent dynamics of electrons, both free or bounded in excitons and trions, has been analysed in semiconductor double quantum wells. In order to study the effect of the different carrier concentrations (electrons and holes) we have performed calculations within the framework of the matrix density formalism. According to the obtained results, we propose a new method to generate trions in coupled quantum wells through injected electrons and holes from doped layers, with an excess of electrons. The excess of free electrons together with the direct created excitons form the trions. This method avoids the undesirable effects coming from the photoexcitation. Due to the effect of trions on the free electron dipole moment, these complex species can be detected through the electromagnetic radiation emerging from the sample after the electron and hole injection.

**S3X7** **Comparison of semiclassical and quantum-mechanical description of 3D semiconductor superlattices subject to tilted magnetic fields**

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*2) I. Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany*

We propose a simple tight–binding fully-quantum-mechanical model of a 3D short–period semiconductor superlattice with one occupied miniband. The model is capable of explaining experimental magnetoresistance data. The 3D Schrödinger equation was reduced to 1D in $\vec{k}$–space and solved both quantum-mechanically and semiclassically for a wide variety of superlattice's parameters, tilt angles and magnitudes of magnetic fields. The solutions determine the region of parameters for which the quantum-mechanical and the semiclassical approaches are significantly differ.

### S3X8 **Photoreflectance from GaAs/GaAsP short period superlattices**

Lev P. Avakyants[1], Pavel Yu. Bokov[1], Anatoly V. Chervyakov[1], Tamara P. Kolmakova[2]
*1) MV Lomonosov Moscow State University, Physics dept, Moscow, Russia*
*2) SII Saphire, Moscow, Russia*

Photoreflectance (PR) spectra of strained GaAs/GaAsP short period superlattises (SL) grown by liquid phase epitaxy with 0.4 phosphorous concentration was registered at room temperature. The following lines were observed at PR spectra: 1.41 eV connected with GaAs substrate, 1.77 eV from strain GaAsP barriers and lines from transition between conductance and valence bands SL minizones. The energies of transitions between conductance and valence bands SL minizones were calculated from Kronig-Peny periodic potential model with taking into account deformation-induced changes at band structure of SL. The best accordance between experimental and calculated data was observed for case 0.2 of band gap GaAs and GaAsP discontinuity fall at conductance band and 0.8 fall at heavy hole valence band, which corresponds to common-anion rule.

### S3X9 **Structures of silicon carbide films on sapphire and graphite**

Y. BabA[1], T. Sekiguchi[1], I. Shimoyama[1], Krishna G. Nath[1]
*1) Japan Atomic Energy Research Institute*

Silicon carbide has attracted much attention as a wide-gap electronic and optoelectronic material due to its chemical stability and high thermal conductivity. Here we report on the structures of thin and thick SiCx films deposited on sapphire and graphite surfaces. SiC films were deposited by ion beam deposition and post-annealing using tetramethylsilane as a source material. The structures of the films were analyzed in-situ by core-level spectroscopy using synchrotron soft X-rays. For thick layers, the structures of deposited films were similar to those of the bulk SiC. For ultra-thin layers, it was found that the films have a flat-lying structure of which configuration is similar to a single sheet of graphite.

### S3X10 **HALL CURRENT IN PLANAR QUANTUM WIRE IN NORMAL MAGNETIC AND ELECTRIC FIELDS**

Niyazi M. Huseynov[1], Seyid-Nisa M. Seyid-Rzayeva[1]
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It is considered a planar quantum wire situated in $x, y$- plane along the $y$-axis in magnetic and electric fields oriented along $z$-axes and $x$-axes correspondingly. A degenerate electron gas is confined in $x, y$-plane by the parabolic potential $m\omega_0^2 x^2/2$, where $m$ is the electron's effective mass. We choose $\omega_0$ such that $m\omega_0^2 d^2/8 \approx E_F$, where $d$ is the width of the wire, $E_F$ is the Fermi energy. The non-dissipative Hall current was calculated. It is shown that the full non-dissipative current is: $J_y = -J_{Hall}/(1 + \omega_0^2/\omega_c^2)$, where $J_{Hall} = -(e^2 n_e E d)/(m\omega_c)$ is the 'standard' Hall current, $e$ is the electron charge, $n_e$ is the two-dimensional density of the electron gas, $\omega_c$ is the cyclotron frequency, $E$ is the electrical field being the sum of the external field and the one arisen in the result of the gradient of the electron's concentration along the $x$-axis. In the case of parabolic potential the influence of the edges of the wire leads to change of orientation of the non-dissipative current. All the electrons take part in formation of the transverse polarization $P = e \sum_{n, x_0} x_0 |\Psi_{n,x_0}|^2 f_{n,x_0}$, defining the difference between $J_y$ and $J_{Hall}$. Where $\Psi_{n,x_0}$ is the electron's wave function, $n$ and $x_0$ are the quantum numbers, $f_{n,x_0}$ is the distribution function. In the case of the more 'hard' walls (for example: in the case of the square well confinement) the only electrons centered near the wire edge (typically within the distance of one cyclotron radius $l$ of the wire edge) feel the wall of the quantum well. For strong magnetic field $l << d$ the deviation of $J_y$ from $J_{Hall}$ is negligible.

S3X11 **Fine structure of Landau subbands in GaAs/AlGaAs three-dimensional superlattices subject to tilted magnetic fields**

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*1) Institute of Physics, Prague, Czech Republic*
*2) Grenoble High Magnetic Field Laboratory, Grenoble, France*
*3) University of Regensburg, Regensburg, Germany*

Tilted field magnetoresistance was measured on MBE-grown GaAs/AlGaAs superlattices, consisting of 30 GaAs quantum wells ($D = 18.8$ nm) separated by Si-doped $Al_{0.3}Ga_{0.7}As$ barriers ($d = 5.1$ nm). Three samples of standard Hall bar geometry have been prepared from different parts of the wafer and both longitudinal and transversal magnetoresistance measured at $\approx 0.4$ K in fields up to 23 T. Within the interval of tilt angles $25° \leq \alpha \leq 52°$, new features could be seen superimposed on the SdH curves just above the minimum corresponding to the filling factor $\nu = 2$, i.e. in the low-field tails of the lowest Landau level. We attribute these new oscillations to the extended "belly" orbits (electrons travel in three wells through two barriers) arising in this interval of angles.

S3X12 **Influence of superconductor transition in vanadium on magnetic state of Fe/V multilayered structure studied by polarized neutron reflectometry**

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The measurements of nuclear and magnetic profiles for the structure Pd(1.5nm)/ V(40nm)/ 17[Fe(0.145nm)/V(0.145nm)]/10[Fe(5nm)/V(5nm)]/MgO placed in magnetic field at temperatures of 1.7, 3 and 290 K were carried out by the method of polarized neutron reflectometry. For temperature of 290 K the magnetisation distribution was detected to be unproportional to iron atom concentration. For the temperature of 1.7 K and at magnetic field of 700 Oe phenomena of 2.5% decrease of iron layer magnetisation, 3 kOe decrease of Fe/V interface magnetisation and 50% magnetisation increase for the structure 17[Fe(0.145nm)/V(0.145nm)] were observed. These data show the magnetisation of vanadium atoms by iron atoms, the influence of superconductor transition on magnetization distribution and the dependence of these phenomena on atom concentration.

S3X13 **Impurity Density of States in Semiconductor Fibonacci Superlattices**

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*2) Departamento de Física, UFRN, 59072-970, Natal-RN, Brazil*

The Fibonacci superlattice (FSL), which is made by juxtaposing two different building blocks A and B arranged in a Fibonacci sequence, has become a standard model for the study of quasiperiodic systems. In this work, we have developed a method to determine the binding energies of a GaAs-(GaAl)As FSL based on Dyson's equation together with a transfer-matrix treatment, within the tight-binding Hamiltonian model. We have calculated also the electronic density of state stressing the region of frequency where the transfer function is complex, corresponding to non-localized states. On the other hand, the localized states are found in the high-frequency region of the electronic spectrum, corresponding to real transfer function and exponentially decaying density of state.

S3X14　**Photoluminescence kinetics of type II GaAs/AlAs superlattices under the influence of an electric field**

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The photoluminescence (PL) kinetics in type II GaAs/AlAs superlattices under the influence of an electric field is reported in this work. We have found that the application of electric field leads to an appearance of e-hh PL line and an increase in the PL intensity of free exciton line. Next, with a delay after the electric field pulse an acceleration of the PL decay of the excitonic lines and phonon replicas is observed. These changes in the PL kinetics dont depend on the electric field pulse duration. We conclude that the electric field ionises donors in the GaAs layers. Some electrons ejected at $\Gamma$-states in the GaAs transfer to the X-states in the AlAs that causes an enhancement of the PL intensity of free exciton and e-hh lines. The rest electrons are heated by electric field and scatter to the X-states in the GaAs. Transiting to the lowest-lying X-states in the AlAs these electrons cause the acceleration of the PL decay due to impact ionization of the excitons.

S3X15　**Excitons in ultra-thin bimolecular crystalline films**

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*2) Faculty of Sciences, Universitiy of Novi Sad, Serbia and Montenegro*

Dispersion laws of Frenkels excitons in perturbed molecular ultra-thin films are found using method of two-time temperature Green's functions. Disturbing of energy parameters on boundaries and space boundaries are considered as perturbations. The cubic crystalline system with complex cell, compound of two molecules (*a* and *b*), i.e. bimolecular film, was analyzed in harmonic approximation. The significant results are that the sharp discrete energetic levels are obtained as well as narrowing of energetic zones. Those results (discretisation and narrowing) are expectable as a consequence of adequate treatment of dimensional quantization or changing characteristics of molecules itself.
We calculate the distribution of exciton states along the *z*-direction in the ultra-thin bimolecular film. Existence of localized exciton states at boundaries are of special interest, considerable depending on energy and/or boundary parameters.

S3X16　**High-temperature quantum oscillations of the impedance of layered conductors**

Olga V. Kirichenko[1], Igor V. Kozlov[1]
*1) B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine*

We have studied theoretically the propagation of electromagnetic waves in Q2D layered conductors placed in a strong magnetic field H. In the case of elastic scattering of charge carriers at impurities account of the quantum oscillations of the scattering operator results in the oscillatory dependence of the impedance on 1/H. These oscillations are formed by the interference of the harmonics with the frequencies determined by the extreme-areas cross sections of the Fermi surface. The temperature smearing of the Fermi function does not lead to a decrease in the amplitude of the low-frequency oscillations determined by the difference between the extreme areas. The low-frequency quantum oscillations of the impedance might be observed at high enough temperatures up to liquid hydrogen temperature.

S3X17 **Electron Raman scattering in parabolic quantum wire in a transverse magnetic field**

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Electron Raman scattering (ERS) are investigated in a parabolic semiconductor quantum wire in a transverse magnetic field. It has been shown, that the energy spectrum depends on hybrid $N_{hyb}$ and size $N_{size}$ quantum numbers. The process involves an interband electronic transition and an intraband transition between quantized subbands. It has been established that the intraband transitions depend on the polarization of incident and scattered radiations, while the interband transitions do not depend on the polarization. We analyze the differential cross-section for different scattering geometry. In the case of interband transitions, there are not selection rules for the hybrid quantum number , but for the size quantum number the selection rule is $N_{size} = 2k$, where $k = 0, 1, 2\ldots$ .In the case of intraband transitions, the selection rules for hybrid and size quantum number are $0, \pm 1$; depending on the polarization. The singularities in the Raman spectra are found and interpreted. ERS cross-section is proportional to the combined density-of-states and the transition matrix element. In this case, the scattering spectrum has singularities related to the combined density-of-states and maxima related to the interband matrix element, and shows strong resonance when scattered frequency equals the hybrid and confinement frequency. The Raman peak shifts towards low energies when the magnetic field increases.

S3X18 **EXPERIMENTAL STUDY OF LOW DIMENSIONAL MAGNET WITH SPATIALLY ANISOTROPIC EXCHANGE COUPLING**

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We present the analysis of specific heat data down to 100 mK and magnetic susceptibility of $Cu(C_{10}H_8N_2)(H_2O)_2SO_4$. The study is motivated by obtaining the information on the nature of magnetic interactions in the material. Detailed inspection of the crystal structure reveal that the interactions Cu(II) can probably be mediated through exchange paths of the $[SO_4]^{2-}$ groups along $c$-direction and the hydrogen bonds in the $b$-direction. Exchange paths might represent a zigzag ladder with spatially anisotropic exchange coupling. Surprisingly weak magnetic correlations observed in the material can be ascribed to the non-trivial magnetochemistry of the hydrogen bonds present in the structure.

S3X19 **Interface structure of metallic multilayers**

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Using first principles calculations we show that the magnetic moment, the critical temperature and the interlayer exchange coupling of magnetic multilayers can be reproduced with good accuracy, provided interface alloying and interface roughness are incorporated. A study was performed specifically for the Fe/V and the $Fe_{0.82}Ni_{0.18}$/V systems, but the interface structure models apply for general metallic multilayer systems. By combining theoretical modelling with experimental results we are able to quantify several features of the interface structure. Most importantly, it was demonstrated that the interfaces for the studied systems, have interdiffusion essentially over 2-3 atomic layers on each side of the interface. We argue that combining experimental work with theoretical modelling is a good avenue to obtain accurate information about the interface quality of metallic multilayers.

S3X20 **Dynamical response at finite momenta and collective excitations in a disordered two dimensional electron system exposed to a perpendicular magnetic field**

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We study the dynamical response at finite momenta and temperatures in a *disordered two dimensional electron system exposed to a perpendicular magnetic field. Electron-electron interaction is treated in the random phase approximation and electron-impurity interaction, in the self-consistent Born approximation with the consistent vertex corrections included. We calculate the real and imaginary parts of dielectric function, the structure factor as well as the spectra of intra- and inter-Landau level collective excitations for different values of electron mobility, density, magnetic field, and temperature.*

S3X21 **ENERGY SPECTRUM OF CARRIERS IN KANE TYPE HOLLOW CYLINDER**

Firudin Gashimzade[1], Arif Babayev[1], Seyfettin Cakmak[2], Sukru Cakmaktepe[2]
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The energy spectrum of carriers confined to a narrow gap semiconductor hollow cylinder with hard walls are calculated both without and with an applied constant axial magnetic field.Taking into account the real band structure of InSb-type materials:narrow energy gap and strong spin-orbit interaction. We calculated the size and magnetic field dependence of effective g-value in bare InSb type hollow cylinder for electrons. It has been seen that the effective g-value of the electrons are decreased with the increasing of radius. The magnetic field dependense of g-factor has a minimum only for subbands with the negative m.

S3X22 **RAMAN SPECTRA OF BISMUTH OXYHALIDE SINGLECRYSTALS**

Victor V. Bunda[1]
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The Raman spectral data of solid state (as a singlecrystals) bismuth oxyhalides have not as yet been extensively studied. In the present study, the Raman active vibrational fundamentals of the singlecrystalline bismuth oxyhalides, BiOCl, BiOBr and BiOI, are discussed using the results of the factor group analysis. The optically active normal vibrations are discussed by comparison with the results of the calculations of phonon spectra in terms of rigid ion model. The BiOHal singlecrystals were grown either by the chemical gas transport reactions method. The bismuth ions have a monocapped square antiprismatic surrounding of four oxygen and five halogen atoms. The Raman active modes are observed in frequency range 55-225; 50-185; 45-175 $cm^{-1}$ for the BiOCl, BiOBr and BiOI singlecrystals, respectively. The halogen substitution effect on the Raman spectra of the BiOHal (Bismocklit family) crystals and the correlations between experimental and calculated results are observed.

S3X23 **Phonon spectra and discrete oscillatory levels in crystal superlattices of deuterium- and hydrogen-palladium solid solutions**

S.B. Feodosyev[1], I.A. Gospodarev[1], V.I. Grishaev[1], A.M. Kosevich[1], O.V. Kotlyar[1], E.S. Syrkin[1]
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Phonon spectra and oscillatory thermodynamic characteristics of PdH and PdD solid solutions are investigated. At high concentration of hydrogen or deuterium atoms one can treat the solutions as a superstructure with random distribution of vacancies in a hydrogen subsystem. Characteristics of the local vibrations of substitutional impurity are calculated for frequencies belong to gap between acoustic and optical zones (D in PdH) as well as for the areas outside the phonon spectra (H in PdD). Closed analytical expressions for local frequencies received in [1] are used to elucidate effect of vacancies in hydrogen subsystem. Diverse configurations of vacancies close to impurity atoms are discussed.
1. O.V. Kotlyar, S.B. Feodosyev, 19th General Conference of CMD, Europhysics Conference Abstract, V. 26A, C22.P.3.7 (2002)

S3X24 **Theory of Negative Differential Resistance and Current-Voltage Asymmetries in Double Quantum Dots**

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An explanation for the negative differential conductance in a double quantum dot system attached to metallic external contacts is proposed, based on a diagrammatic technique for non-equilibrium many-body operator Green functions. The theory suggests that tunneling between the states in the double quantum dot suppress the total current dynamically as the bias voltage is increased. The effect is especially evident in systems where the double quantum dot states are asymmetrically coupled to the left and right contacts. The suggested theory also explains the commonly observed current-voltage asymmetries in mesoscopic multilevel systems. Our theory is consistent with recent experimental data on double quantum dots.

S3X25 **Disordered magnetic multilayers: Electron transport within the CPA**

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In this work we calculate on an ab initio level spin-dependent transport properties of metallic magnetic multilayers in the CPP geometry, which allows us to study the giant magnetoresistance ( GMR ) phenomena. One of the main problems is to deal with substitutional disorder, which comes from alloying in layers or from the inevitable interdiffusion at interfaces. In existing works based on ab-initio calculations this was usually solved using a supercell method. An alternative way is to use the coherent potential approximation ( CPA ). In our calculations we employ the full CPA for the transport including its difficult part, namely vertex corrections, which are neccesary to obtain two-particle properties like conductances. In this way we obtain ballistic as well as diffusive part of the electron transport. Our results show remarkably good agreement with experiments, while the computational requirements remain modest.

**S3X26** **Resonance heat transport between two solids through multiplayer interface**

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Experimentally observed solid-solid thermal resistance shows essential features. The mechanism of the resonance transport of phonons considered in the present work is characteristic for heat transmission between two media. In point contacts molecules of water or solidified inert gases can serve as a resonance layer. Peaks of the reduced heat flow considered in the present work are observed, for example, in KBr-KBr, KBr-Cu. In these contacts a low-temperature maximum observed can be explained by the theory of the resonance transport. Multichannel resonance transmission of phonons through the interface of the point contact Si-Cu was studied using the capillary effects theory. The results obtained are in a good agreement with the experimental data.

**S3X27** **ESR INVESTIGATION OF MONOCLINIC SINGLET $KTb(WO_4)_2$**

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Potassium terbium double tungstate $KTb(WO_4)_2$ belong to the family of double alkali rare earth tungstates. $KTb(WO_4)_2$ refers to the monoclinic space group 2C/c. The unit cell contains four molecules. The rare-earth ions form chains along face diagonal [101]. The ground state of ion $Tb^{3+}$ is $^7F_6$. In the range of temperatures $1,8 - 300$ K the crystal is paramagnetic. High frequency properties of $KTb(WO_4)_2$ was studied at temperatures 1.7 - 4.2 K in frequency range 1.8 - 120 GHZ in permanent magnetic field up to 8 T. The energy gaps between lowest electron levels and g- factors of the ground state was determines ($\Delta E_1 = 0,65 \pm 0,05$ cm$^{-1}$ $\Delta E_2 = 2,2 \pm 0,05$ cm$^{-1}$; $\Delta E_3 = 3,07 \pm 0,05$ cm$^{-1}$; $g_1 = 14$; $g_2 < 0.5$; $g_3 < 0,5$). When external field is applied perpendicular to chains direction a structural first kind phase transition induced by an magnetic field was detected in field 34.5 kOe. Phase transition is going through an incommensurate phase.

**S3X28** **SPIN-PLASMA WAVES IN 1D-METAL**

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It is shown that a new type of weakly damping acoustic plasmons may propagate in a quazi-one-dimensional conductor placed in an external constant magnetic field. Such waves are caused by presence of spin subbands in electron energy spectrum and so have to be accompanied by forced oscillations of a magnetic moment of the sample. Magnetic field dependences of the velocity and amplitude of these waves are obtained. In principle the effect can be used in constructing adjustable wideband delay lines for electromagnetic signals.

**S3X29** **The cyclotron waves in layered conductors under strong spatial dispersion**

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The propagation of electromagnetic waves in layered conductors with the quasi-two-dimensional electron energy spectrum at the presence of an external magnetic field $\mathbf{H_0}$ is investigated theoretically. At some orientations of a magnetic field about the layers of the conductor the drift velocity of electron $v_H$ along the direction of $\mathbf{H_0}$ is close to zero. For these directions of $\mathbf{H_0}$ the collisionless absorption is absent and weak damping waves can propagate even under the conditions of strong spatial dispersion. In a short-wave limit the existence of electromagnetic waves with frequencies near the cyclotron resonance is possible at an arbitrary orientation of the wave vector $\mathbf{k}$ with respect to $\mathbf{H_0}$. In quasi-isotropic metals the similar types of waves take place only when $\mathbf{k}$ is perpendicular to the direction of a magnetic field.

**S3X30** **Non-linear electron transport in weakly-coupled disordered semiconductor superlattices**

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We study theoretically vertical electron transport in weakly-coupled semiconductor superlattices. Sequential tunneling between adjacent quantum wells in the presence of phonon and impurity scattering is considered. Kinetic and Poisson equations are solved self-consistently regarding the electron concentrations and well potentials. A proper description of the contact phenomena is proposed. Effects of the disorder in the layer parameters on the stationary current-voltage characteristics are summarized. We derive analytically the conditions for the observation of Z-shaped $I$-$V$ curves, which are valid for any electron transition rates of resonant nature. Disorder-induced transitions between N- and Z-shaped current maxima are investigated. The possibility to control the electrical properties of superlattice by the disorder is discussed.

**S3X31** **Dimensional resonances of elastic and magnetoelastic waves in layered structure**

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Peculiarities of dimensional resonances of elastic and magneto- elastic waves in bi-layered insulator structure: ferromagnetic film - non-magnetic elastic substrate have been investigated. Excitations are generated by driving magnetic field. At a definite ratio between driving field frequency and dimension of double layered structure thickness vibration modes are observed. Dependences of resonant frequencies of vibration modes upon thicknesses of magnetic and non-magnetic layers, elastic and magnetoelasic parameters, applied magnetic field have been calculated. Presence of peculiarities of resonant frequencies harmonics behavior at the change of magnetic layer thickness have been shown. The dimensional resonance frequency f reveals non-monotonic dependence on the magnetic layer thickness d. The shape of the curve describing dependence f(d) becomes a function of wave resistances of two mediums. The non-monotone behavior of frequency of composed structure results in inharmonic arrangement of resonant frequencies. Comparison of theoretical calculations with experimental measurements has been presented.

**S3X32** **Coulomb drag near the metal-insulator transition in two-dimensions**

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We studied the Coulomb drag between dilute two-dimensional hole systems in the vicinity of the apparent metal-insulator transition. Our measurements range from densities of 7.0 to below $1.0 \times 10^{10}$ cm$^{-2}$. We find that in this regime the drag exhibits a 2 to 3 order of magnitude enhancement over that expected from Boltzmann theory. In addition, significant deviations to the expected $T^2$ dependence are observed, with these deviations correlated with the metallic behavior in the single layer resistivity. Furthermore, the spin polarization dependence of the drag has been investigated by applying an in-plane magnetic field. Here we find that the magnetodrag and the single layer magnetoresistance exhibit the exact same qualitative features. These results will be discussed in light of interaction effects and screening in this dilute regime.

### S3X33    The high-temperature quantum size effect in thin metal films.

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High-temperature quantum oscillations (QHTOs) of the conductivity in thin metal films are theoretically investigated. The case of the thin metal film with mirrorlike boundaries and two groups of charge carriers (electron and hole) is considered. It is shown that in the case of elastic scattering by impurities there occur QHTOs of the conductivity weakly insensitive to the temperature smearing of Fermi level. The influence of the unequal spacing of the energy spectrum on the frequency of the size oscillations and the character of the temperature dependence of the QHTOs are investigated.

### S3X34    Polaron exciton spectra in quantum dots.

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In quantum dots based on semiconductors with high ionicity, the optical transition into the polaron exciton state is accompanied by the electron and hole polarization of the medium. The polaron effect in quantum dots results in multiple phonon replicas of the exciton optical transition line. It is shown in this paper that in the spherical quantum dot the polaron exciton under the strong confinement regime creates anisotropic polarization of the medium. Nevertheless the polarization does not split of the degenerate ground state of the polaron exciton. The average value of exciton angular momentum component $J_z$ vanishes, $\langle J_z \rangle = 0$. The emitted light from spherical dot is not polarized. The picture is different in a case of ellipsoidal quantum dot. The ground state of the hole in ellipsoidal quantum dot is split into the states with the hole angular momentum components $J_z^{(h)} = \pm 3/2$ and $J_z^{(h)} = \pm 1/2$. The light emitted from ellipsoidal dot has the specific polarization. The study enables us to make a conclusion on the quantum dot geometry.

### S3X35    High-field magnetoelastic behavior of $PrCo_2Ge_2$ single-crystal

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The single crystal of novel tetragonal $PrCo_2Ge_2$ compound has been grown; characterized by X-ray powder diffraction and studied in detail by means of magnetization (M) and dilatometric (dl/l) measurements in a temperature range 2-300K and magnetic fields up to 14T. The compound orders antiferromagnetically at $T_N \sim 28K$ and exhibits an additional order-to-order magnetic phase transition at $T_1 \sim 8K$ as determined from M(T) dependency. The pronounced magnetocrystalline anisotropy is present in this compound. The cascade of two metamagnetic phase transitions has been observed on the M(H) and dl/l(H) curves measured at 2K in magnetic field applied along the c axis (easy magnetization direction) at $\sim$ 2T and 11T, respectively.

S3X36 **Tunnel junctions with charge-density-wave metals in magnetic fields**

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Voltage-, $V$,dependences for tunnel conductances $G$ for junctions in a magnetic field $H$, involving metals partially gapped by charge-density waves (CDWMs), are calculated. When one electrode is a normal metal, the peaks of $G(V)$ determined by the dielectric gap $\Sigma$ are split similarly to as if the CDWM electrode were a superconductor. The results differ from those in the latter case. If the electrode is ferromagnetic, $G(V)$ depends on its polarization $P$. Equations for the general CDWM–CDWM$'$ set-up are derived. Since there are nested and non-nested sections of the Fermi surfaces, the $H$-induced splitting exists in this case, contrary to what is observed when the sandwich covers are superconductors. This phenomenon may serve as an indicator of the CDW appearance.

S3X37 **Influence of the growth parameters on the Curie temperature of La$_{0.7}$Sr$_{0.3}$MnO$_3$ half-metallic films**

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La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) thin films have been successfully employed in Magnetic Tunneling Junctions displaying very high values of the Tunneling Magneto Resistance at 4K. Despite the relatively high Curie temperature (Tc) of bulk LSMO (370 K), spin dependent transport phenomena are strongly reduced at room temperature, due to the reduced Tc at surface. We have systematically investigated the influence of various growth parameters in LSMO/SrTiO$_3$(001) thin films grown by PLD, on the Tc and on the temperature Tp at which the metal-insulator transition takes place. We found that a high Tc and room temperature magnetisation can be obtained increasing the mobility of clusters on the substrate and allowing the system for long diffusion times between subsequent laser pulses. This fact is accompanied by a sizable increase of Tp that can exceed Tc by 80K.

S3X38 **NiFe$_2$O$_4$ : a new material for spintronics**

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An interesting route to develop new materials for spintronics is doping semiconductors (GaAs, ZnO) with a 3d element. Here, we propose an alternative method : we grow ultrathin films of a ferrimagnetic insulating spinel (NiFe$_2$O$_4$) and show that, in specific conditions, the films exhibit a greatly enhanced magnetic moment and a conductive behavior. As a result, our films can be used as electrodes in magnetic tunnel junctions. We report on the observation of a TMR of 120% at 4K in La$_{2/3}$Sr$_{1/3}$MnO$_3$/SrTiO$_3$/NiFe$_2$O$_4$ junctions. This corresponds to a spin-polarization of 40% that is conserved up to 300K.

S3X39 **METAL-DIELECTRIC TRANSITION IN IRRADIATED $La_{0.85}Sr_{0.15}MnO_3$ SINGLE CRYSTAL**

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Behavior of resistance $\rho(T)$ and ac magnetic susceptibility $\chi(T, H = 0)$ was studied for perovskite lanthanum manganite $La_{0.85}Sr_{0.15}MnO_3$ single crystal irradiated by neutrons of $2 \cdot 10^{19} cm^{-2}$ fluence and annealed at temperatures from 200 to 1000 C. As it was observed the $\rho(T)$ irradiation leads to disappearing of the low temperature dielectric phase. Increasing of the annealing temperature does not recover the insulating phase in the sample but raises the transition into a metallic-like state. According to the $\chi(T, H = 0)$ behavior irradiation leads only to decreasing of the paramagnetic to ferromagnetic transition temperature $T_C$ and the susceptibility value. Annealing temperature increasing involves rising as $T_C$ as the susceptibility value to the values in the not irradiated sample. The observed difference in the electrical and magnetic properties in the irradiated $La_{0.85}Sr_{0.15}MnO_3$ single crystal is explained qualitatively.

S3X40 **Metal-insulator transition in graphite.**

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The features of the transport properties and metal-insulator transitions (MIT) in the highly ordered pyrolytic graphite have been experimental investigated at the temperature from 0,3 to 150 K and magnetic field up 9 T for the magnetic field applied parallel to c-axis. The measurements of resistance show that R(T) demonstrated a maximum at field-dependent temperature - $T_c$; in the interval from 300 mK to $T_c$- metallic behavior of resistance; in the interval from $T_c$ to 135 K - insulator-like behavior of resistance. The Hall measurment have shown that at T=300 mK the minima in the Shubnikov-de-Haaas oscillations correspond to 0,58, 0,64, 0,74, 0,87, 1,07 and 1,38 T. The MIT appears with increase of the magnetic field (up to 9 T) in the temperatur interval between 17 and 21 K.

S3X41 **Optical properties of solids in extreme conditions using far-infrared brilliant synchrotron radiation sources**

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In the last decade many infrared beamlines have been installed at existing synchrotron radiation facilities and new important opportunities are now offered by these unique infrared sources in solid state physics. In 2003 has been completed the commissioning of SINBAD, the first Italian infrared beamline, now operational at DAFNE, the storage ring of the Laboratori Nazionali di Frascati of the INFN. Both the high electron beam current, up to 1.8 A, and its low energy of 0.51 GeV are ideal parameters for the infrared synchrotron radiation emission. SINBAD covers the entire IR range, from 10 to 10000 cm-1 with a brilliance gain compared to a standard source of about 30-40 times in the far-IR range. High-resolution FTIR spectroscopy can be performed using a modified Bruker Equinox 55 interferometer working in vacuum. Moreover, a Bruker IRscope I microscope has also been installed and is operational in both the near-IR and the mid-IR ranges. We present the first data of FTIR spectroscopy and micro-spectroscopy collected at SINBAD in these first months of operation. Special emphasis will be given to the investigation of far-IR transmission spectra of colossal magnetoresistance manganites (La1-xCaxMnO3) at high pressure, using a diamond anvil cell at room temperature. Far-IR synchrotron radiation spectroscopy is indeed a powerful tool for the investigation of insulating-to-metal transitions and charge ordering phenomena that occur in these oxides.

S3X42 **Rashba Spin Double Refraction in Heterostructures**

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The Rashba spin-orbit coupling in a two dimensional electron gas gives rise to a double refraction phenomenon in which the spin behaves like the polarization of light in a biaxial crystal. We demonstrate how this spin-orbit coupling in semiconductor heterostructures can produce and control a spin polarized current without ferromagnetic leads. The effect can be regulated by a couple of narrow Quantum Point Contacts, that control the input incidence angles of the electrons entering into the barrier where the spin-orbit coupling is confined. There is a limit incidence angle at which one of the two modes of propagation within the barrier is totally reflected and this event shows up by the halving of the quantized steps of the conductance. This feature could be used as an experimental signature of spin double refraction. We present a detailed study of the spin polarization of electrons exiting from the barrier. The double step of the transmission coefficient remains also when the two Quantum Point Contact are decoupled assuming that the barrier is so large that the phase coherence is maintained only for a single crossing of the barrier. 1)V. Marigliano Ramaglia, D. Bercioux, V. Cataudella, G. De Filippis, A.C. Perroni and F. Ventriglia, Eur.Phys.J. B 36, 365 (2003) 2)M.Khodas,A.Shekhter and A.M.Finkel?stein, Phys.Rev.Lett. 92, 086602 (2004) 3)V. Marigliano Ramaglia, D. Bercioux, V. Cataudella, G. De Filippis, A.C. Perroni, cond-mat/0403534 22/03/2004

**S3X43** **Interplay of charge transport and magnetization in electronic devices with a single-molecule magnet**

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Single-molecule magnets(SMMs) have been investigated as molecule-scale unit for information storage or qubit for quantum computation. This goal can be realized by depositing SMM on a suitable metal and probing it using scanning tunneling microscopy, or by making a break junction with SMM. However, before designing real experiments, it is desirable to study theoretically the interplay between charge transport and the magnetic properties of SMM in such electronic devices. In this work electronic transport will be theoretically studied in such systems. Employing the exchange model and the Landau-Zener model, we present stepwise behavior of the linear response conductance with increasing longitudinal field and oscillatory structures at each step as a function of the transverse magnetic field along the hard axis.

**S3X44** **Spin dynamics in the vicinity of the field-induced quantum critical point in a quasi-two-dimensional antiferromagnet**

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Spin dynamics in an insulating layered non-collinear anitiferromagnet Pr2CuO4 have been studied by inelastic neutron scattering in magnetic field near the quantum critical point at Hc = 3 Tesla (T = 0 K). With a magnetic field applied along the crystallographic direction [110], the spin structure undergoes a second order phase transition with one vanishing component of the two-component order parameter with the line of the phase transitions Hc(T) ending, at T = 0, at the quantum critical point. We have observed that in approaching the critical field the lowest energy gap at the magnetic Brillouin zone centre is filled up with states so that at the critical field no gap can be observed within experimental resolution (0.1 meV). At higher fields the spin-excitation gap opens again. The results will be discussed in the light of recent theoretical developments.

**S3X45** **Resonant magnetopolaron coupling of an interacting polaron gas in a quantum well**

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Cyclotron-resonance spectra of a gas of interacting polarons confined to a GaAs/AlAs quantum well in the presence of a tilted magnetic field are theoretically investigated taking into account the magnetoplasmon-phonon mixing. The resonant magneto-polaron coupling in a high-density GaAs/AlAs quantum well occurs near the GaAs TO-phonon frequency rather than near the GaAs LO-phonon frequency both in normal and tilted configurations. We interpret the effect of the shift of the anticrossing point from $\omega_{LO}$ to $\omega_{TO}$ in terms of the resonant coupling of the electrons with the mixed magnetoplasmon-phonon modes. Calculated CR spectra are in agreement with recent experimental data. This work has been supported by the GOA BOF UA 2000, IUAP, FWO-V projects G.0274.01N, G.0435.03, the WOG WO.025.99 (Belgium) and the European Commission GROWTH Programme, NANOMAT project, contract No. G5RD-CT-2001-00545.

S3X46 **Revelation of negative magnetoresistance in YbFe$_4$Al$_8$.**

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The surface resistance R$_S$ of three polycrystalline samples of YbFe$_4$Al$_8$ was investigated at a frequency 30 MHz in low magnetic fields (0-100 Oe) and in the wide temperature range (300-4.2 K). The surface resistance was measured by a contact-free resonator method. The anomalous extremum of R$_S$ was found within the temperature range 57-35 K with the maximum located at T$_{max}$ = 50 K in all samples. The low magnetic fields (5-50 Oe) suppress this extremum, revealing the negative magnetoresistance. In the magnetic field H=50 Oe the values of relative magnetoresistance reached of 3.5% and didn't change while the magnetic field increased from 50 Oe until 100 Oe.

S3X47 **Spin Polarized Inverse Photoemission from Fe$_3$O$_4$(111)**

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Magnetite (Fe$_3$O$_4$) has been predicted to be half-metallic in the bulk and has a high Tc, which make it a promising candidate for the use in Magnetic Tunneling Junctions. We grow single crystal magnetite films with (111) free surface by MBE on Al$_2$O$_3$ with a Pt(111) buffer layer. The samples are characterized by XPS, Optical and Atomic Force Microscopy, LEED and MOKE for chemical, structural and magnetic properties. We present the first magnetic characterization of the unoccupied electronic structure above E$_F$ performed by angle resolved Spin Polarized inverse Photoemission. The results shed light over the electronic structure determining the spin dependent transport phenomena in the direction perpendicular to the (111) surface.

S3X48 **Semiclassical theory of weak antilocalization in ballistic systems**

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We propose a semiclassical theory of weak antilocalization in clean ballistic systems. Our approach is based on the semiclassical Landauer formula that we extended to include spin-orbit interaction. The general theory is applied to chaotic and integrable billiards with Rashba interaction. We find that the spin relaxation in the chaotic systems is qualitatively different from that in the integrable systems. As a consequence, one expects different scales of the weak antilocalization in these cases.

S3X49 **Phenomena in the dynamics of magnetic microparticles: the Zipf-Mandelbrot relation and the anomalous diffusion**

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The magnetic holes system is a fruitfly model for studying cooperative dynamical processes. By varying the frequency and the anisotropy of the external elliptically polarized magnetic field, a variety of phenomena has been observed and are yet to be explored. Here we present a study of a few-body system giving rise to an intermittent behavior consistent with the Zipf-Mandelbrot relation and the anomalous diffusion.

The magnetic holes system is realized by dispersing uniformly sized polystyrene spheres with diameter 50 $\mu$m in a kerosene-based ferrofluid and confined to a 100 $\mu$m thin layer. The external magnetic fields induce an apparent magnetic dipole moment on the microparticles, where all moments have equal strength and direction. The microparticles trace out complicated patterns when subjected to varying external magnetic fields.

S3X50 **Magnetic transitions and magnetocaloric effect in $RE\mathrm{Co}_2$ ($RE$ = Er, Ho) and $RE(\mathrm{Co}_{1-x}\mathrm{Si}_x)_2$ compounds**

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Heat-capacity measurements have been performed on cubic Laves-phase compounds $RE\mathrm{Co}_2$ ($RE$ = Er, Ho) and $RE(\mathrm{Co}_{1-x}\mathrm{Si}_x)_2$ with $x$ = 0.05 in magnetic fields up to 8 T. Anomalies observed in the specific heat indicate first-order magnetic phase transition at the Curie temperature ($T_C$). The total entropy change and the magnetocaloric effect have been evaluated for selected magnetic fields and discussed in terms of the localized $RE$ $4f$ magnetic moments and Co $3d$ spin fluctuations. The substitution of Co by Si enhances $T_C$ for both compounds and reduced the specific heat and total entropy anomaly at $T_C$.

S3X51 **High-field magnetostriction of the valence fluctuating compound YbInCu$_4$**

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The magnetostriction (MS) and magnetization of the YbInCu$_4$ compound with a first-order valence transition have been measured in magnetic fields up to 40 T. It was found that the volume MS at the field-induced transition $\Delta\omega$=-4.5$\times10^{-3}$ corresponds well to the spontaneous volume change at the temperature-induced transition. The magnetovolume coupling constant is large for the mixed-valence state, but strongly suppressed in the local-moment state. The anisotropic MS at the transition reaches $0.8\times10^{-3}$. The temperature and field variations of the anisotropic MS are described well with a single-ion theory. The anisotropic coupling is nearly the same for the mixed-valence and the local-moment state. Perhaps, the scheme of the $J = 7/2$ multiplet level splitting of Yb remains unchanged in the mixed-valence state in spite of a strong coherent Kondo interaction.

S3X52 **4f electron contribution to conductivity of R-Co intermetallic compounds in**

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The determination of the electronic structure of the intermetallic compounds of rare-earth (R) and 3d-transition metals is a nontrivial problem. It is resulted from the fact that in these compounds there are both itinerant (s, p, d) and completely localized (4f) electrons. In many works, the electronic structure of rare-earth metals and of mentioned compounds has been considered in the framework of the one electron approximation not involving the 4f electrons in scheme of energy bands. However certain of workers suppose that the large correlation of 4f electrons is no bar to the involvement of states of these electrons in band calculations. As obtained earlier, the equatorial Kerr-effect spectra are sensitive to the rare-earth component of R-Co intermetallic compounds. Therefore the magneto-optical technique can be used for probing theoretical band models of these compounds. In this paper, we present the spectra of the absorptive part both of the diagonal element $\sigma$xx and of the off-diagonal element $\sigma$xy of the conductivity tensor of DyCo5 and NdCo5 compounds keeping in mind that these quantities are related to the density of electron states derived from band calculations. Data cover the 1-5 eV range of photon energy at room temperature. The spectra are discussed treating the 4f electrons of these compounds as ordinary valence electrons for which the correlation energy is significant. Observed distinctions in the spectral behaviour of the absorptive part of $\sigma$xy for DyCo5 and NdCo5 are explained as resulting from distinction between the densities of conductivity electron states in these compounds due to the fact that in NdCo5 the unoccupied 4f states (4f subband) are superimposed on the minority spin subband of the conductivity electrons. The absence of such superposition for DyCo5 follows from the different magnetic coupling of Dy and Nd with Co in these compounds (contrary to Dy, Nd is ferromagnetically coupled with Co).

S3X53 **Influence of light on magnetic and transport properties of thin manganite films with praseodymium**

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The influence of light on magnetic and transport properties of $Pr_{0.6}La_{0.1}Ca_{0.3}MnO_3$ epitaxial thin films was investigated. It was found that the ferromagnetic metal phase is stimulated by light illumination. The photoinduced increase of volume of ferromagnetic phase is accompanied with decreasing of the field of the ferromagnetic dielectric antiferromagnetic metal phase transition. The illumination by light of the films in magnetic field leads to the drastic decreasing of their resistance and induces the transition to the ferromagnetic metallic state.

**S3X54** **Spin Transport in ferromagnetic insulating bismuth manganite heterostructures**

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We report on the development of a new kind of all-oxide $SrTiO_3//La_{2/3}Sr_{1/3}MnO_3$ (LSMO)/$SrTiO_3$/$La_{1-x} Bi_x MnO_3$ (LBMO)/Au magnetic tunnel junctions in which the insulating barrier (LBMO), is ferromagnetic for spin filtered tunnel transmission. Spin-filtering barrier with a single ferromagnetic metallic electrode (LSMO) is expected [1] to induce a tunnel magnetoresistance (TMR). In our communication, we will describe the growth of LBMO epitaxial films on $SrTiO_3$ substrates, and we will report and discuss the observation of a substantial TMR. [1] P. LeClair et al Appl Phys. Lett. 80, 625 (2002)

**S3X55** **First principles study of the half-metal to metal transition in magnetite**

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We analyze the influence of conditions (stress, substitutional dopants) that induce a half-metal to metal transition leading to a loss of the material's desirable half-metallic properties. Total energies, electronic structure, and magnetic moments are calculated by DFT using the FP-LAPW method. Results obtained within the generalized gradient approximation show excellent agreement with experimental findings. In response to uniaxial, biaxial or triaxial pressure, a half-metal to metal transition occurs, which shifts the Fermi energy from the gap of the majority-spin electrons under the top of the valence band so that both spin channels become metallic. We also performed a analysis of different structural and spin configurations simulating the substitution $Fe_{2.5}X_{0.5}O_4$ (X = Mn, Co, Ni). The Mn-doped crystal is metallic whereas Co- and Ni-doped ones are half-metallic.

**S3X56** **Termination effect on half-metallicity of $Co_2MnSi(001)$ surface**

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The magnetic half-metal Heusler alloy $Co_2MnSi$ is a promising candidate to be possibly relevant as spin injector in new spintronic devices. But there are indications that thin films of this alloy may loose the half-metal character. We have performed DFT calculations using the full potential linearized augmented plane wave method to study the electronic and magnetic properties of a $Co_2MnSi(001)$ thin film at different terminations. Analysing variuos surface termination and capping we find that a Mn cap layer leads to very good spin polarization at the Fermi level. Stability of various terminations will be discussed within the framework of ab initio atomistic thermodynamics. The obtained phase diagram shows that terminations by either Mn or Si atoms (or both) can be stable.

S3X57 **Magnetotransport in dilute 2D Si-MOSFET system**

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The magnetoresistivity of Si-MOSFET 2D system owned to thermoelectric Peltier and Seebeck effects ffor 2D metal-insulator transition regime is calculated [1]. The analysis has been made for arbitrary magnetic field. The parallel magnetic field component, if fixed, results in the spin polarization, and, then the beating pattern of Shubnikov-de Haas oscillations [2]. The tilted field geometry case with the sample rotated in a constant magnetic field [3] is considered for both the partially and spin-polarized 2D system. In absence of the parallel field, low-field magnetoresistivity exhibits SdH beating pattern associated with the valley splitting in Si-MOSFET system. Zero-field valley splitting is estimated. Within Quantum Hall regime, the magnetotresistivity of extremely dilute 2DEG closed to metal-insulator transition is investigated [1]. This work was supported by RFBR and LSF. [1] M.V.Cheremisin, cond-mat/0310769 [2] V.M.Pudalov et al,Phys.Rev.Lett., 88, 196404, 2002 [3] S.A.Vitkalov et al, Phys.Rev.B, 64, 073101, 2001

S3X58 **The effect of milling time on thermal and magnetotransport properties of mechanically alloyed cobalt-copper powders**

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Thermal and structural properties of mechanically alloyed $Co_{30}Cu_{70}$ powders of various milling times are analysed using differential thermal analysis (DTA) and X-ray differaction (XRD) respectively. Room temperature magnetoresistance (MR) measurements are performed on the compressed powders in 11 kOe-field. According to XRD results, all samples consist of Co (hcp), Cu (fcc) and CoO (fcc) phase. The sample milled for 30 hours shows an exothermic transition below $400^oC$ because of the gradual decomposition into cobalt and copper clusters. The sample milled for 60 hours exhibits the largest 10% MR. The smallest MR is obtained from the sample milled for 120 hours whose DTA peak processed the least area. It is likely that the prolonged milling time gives rise to the cobalt-copper solid solution and reduces MR as a result.

S3X59 **Spin-galvanic effect under tunneling through semiconductor barriers**

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The problem of electron tunneling through semiconductor barriers grown of zinc-blende-lattice semiconductors is studied. It has been shown that the Dresselhaus k-cubic spin-orbit splitting of the conduction band results in a dependence of the tunneling transparency of the structure on the electron spin and wavevector. The effect of spin-dependent tunneling can be employed for injection and detection of spin-polarized carriers: (i) electric current flow in the interface plane leads to spin polarization of the transmitted carriers, (ii) transmission of the spin-polarized carriers through the structure is accompanied by generation of an interface electric current. The theory of such 'tunneling spin-galvanic' effects has been developed for symmetrical single barriers and resonant double-barrier structures based on zinc-blende-lattice semiconductors.

**S3X60** **Current Driven Domain Wall Motion in Magnetic U-pattern**

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We have studied the current induced domain wall motion by using patterned U geometry. The observation of two magnetic states of U pattern was evidenced. One is the continuous magnetic state without wall which was stabilized before switching field and the other is the head to head domain wall at the turn area of the U pattern which appeared at field larger than switching field. We investigated the influence of the dc current injection on domain wall motion before switching field. The field deviated to switching field versus dc critical current was fitted linearly by two steps. The critical current varied dramatically as the field close to the switching field and then gradually as the field far away from switching field. These results were also modeled and related to the angles between polarized spins and local moments in spin-transfer effect. Also, the experimental results can be fitted to certain angles that were estimated theoretically. The direct observation of the current driven domain wall displacement was also proved.

**S3X61** **Theoretical investigation of epitaxial growth of Mn on Si(001)**

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Ferromagnetic Mn/Si(001) thin films could be used for spin injection through the metal-semiconductor interface, as required for spintronics devices. We use first-principles calculations (DFT with GGA-PBE and the FP-APW+lo method) to investigate the possibility of ferromagnetic film growth. The calculated potential energy surface for Mn shows that the subsurface interstitial site is most stable. The diffusion of Mn parallel to the Si dimer rows is faster than perpendicular. With deposition of more than 0.5 ML Mn, the Si dimers break and the surface shows a $(1 \times 1)$ structure. Further deposition leads to Volmer-Weber growth of a Mn-Si sandwich structure, stabilized due to the strong Mn-Si covalent bonds. From our study of various silicide compounds, we conclude that the most likely stoichiometry of the epitaxial islands is MnSi in CsCl structure, because this minimizes mismatch strain. Mn-Si sandwiches with two or less layers are found to be ferromagnetic, and show a spin polarization at $E_F$ as high as 50%.

**S3Y101** **Temperature dependence of the trapped field in MgB$_2$ bulks**

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Temperature dependencies of the trapped magnetic field have been calculated for two MgB$_2$ samples prepared by two different techniques: high-pressure sintering and hot pressing. Experimentally measured trapped field values for the first sample coincide remarkably well with calculated ones over the whole temperature range. This shows, on one hand, the validity of the introduced calculation approach, and demonstrates, on the other hand, the great prospects of the hot pressing technology for large scale superconducting applications of the MgB$_2$.

S3Y102 **Why the prediction by Abrikosov crystalline long-rang order of vortex lattice does not correspond to the facts.**

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The distinguished work by A.A. Abrikosov awarded of the Nobel Prize in Physics for 2003 not only has determined the orientation of all investigations of the mixed state of type II superconductors during forty years but also has provoked a mass delusion. It predicted two long-rang order, phase coherence and crystalline long-rang order of vortex lattice, although only phase transition is assumed always on the way from the Abrikosov state in the normal state. Fluctuation theory and experiment [1] show that the prediction crystalline long-rang order does not correspond to the facts [2].
[1] A.V. Nikulov et al, Absence of the Transition into Abrikosov Vortex State of Two-Dimensional Type-II Superconductor with Weak Pinning, Phys.Rev.Lett. 75, 2586 (1995)
[2] A.V.Nikulov, Why Vortex Lattice Melting Theory is Science Fiction, cond-mat/0312641

S3Y103 **Specific heat of selected $AnTGa_5$ compounds**

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The discovery of superconductivity in $PuCoGa_5$ [1] and $PuRhGa_5$ [2] compounds has raised a great interest, positioning actinide materials as a possible new class of superconductors. We present here specific-heat data of selected $AnTGa_5$ (An = U, Pu, Am, T = Co, Rh) with special emphasis on the estimation of the lattice contribution to the specific heat. It is essential for the determination of the Sommerfeld coefficient $\gamma$. The value obtained by such analysis in $PuCoGa_5$ reaches 130 $mJmol^{-1}K^{-2}$, higher than previous estimation [1]. We follow also the changes of the height of the $C_p/T$ jump at the critical temperature when substituting different $An$ and $T$ elements in $PuCoGa_5$, and compare this development to the $\gamma$-value changes.
[1] J. L. Sarrao et al., Nature 420 (2002) 297.
[2] F. Wastin et al., J. Phys.: Condens. Matter 15, 2279 (2003).

S3Y104 **X-ray diffraction study of MgB2 at low temperatures.**

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We have performed powder x-ray diffraction of MgB2 superconductor between 10 and 300 K. Integrated intensity of both (002) and (110) x-ray reflections shows a peak at around Tc, superconducting transition temperature. The integrated intensity of the x-ray reflection is related to the phonon frequency through a Debye-Waller factor. The increase of the reflection intensity can be understood by the hardening of the lattice at around Tc.
Lattice parameters a and c show negative thermal expansion at low temperatures. The negative thermal expansion may have no relation to the superconduting transition and might be due to the electronic origin.

S3Y105 **Magnetic imaging of a drilled YBCO crystal.**

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YBCO single crystals can be successfully drilled without destroying the integrity of the material. A M.O. observation of magnetic field (m.f.) was performed using a ferromagnetic Bi-doped YIG thin film with in-plane anisotropy. The field was perpendicular to the sample surface. We analysed the field maps obtained increasing m.f. and after removal of the stimulus. Flux profiles show the ring shaped sample connected up to 0.2 T. An independent test of flux penetration inside the hole was made at low m.f. by a SQUID.

S3Y106 **Investigations of phase and microstructure development in Bi2223/Ag superconducting tapes by means of high energy X-ray diffraction**

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The influence of heating rate and sintering temperature on the phase and texture development in Bi2223/Ag tapes have been studied in-situ by means of synchrotron radiation. The evolution of the Bi2223 phase content follows a sigmoidal shape for all the studied conditions but the kinetics are influenced by the heating rate used for reaching the reaction temperature. On the other hand, the development of preferential orientation of both Bi2212 and Bi2223 plate-shaped crystallites is more influenced by the reaction temperature than by the heating ramp. Several models are tested for analysing the Bi2223 phase formation kinetics. The results are compared with previously published data.

S3Y107 **Resistive transition in bi-layer superconducting systems**

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We discuss the superconducting transition in systems made from two magnetically coupled layers at zero external magnetic field. The two lowest excitations are *i)* stacks of pancake-vortices and *ii)* pancake vortex-antivortex pairs in the individual layers. Stacks involve a finite, although large, self energy and are present at any finite temperature. The putative Kosterlitz-Thouless transition at which pancake-vortex pairs unbind describes the evaporation of the vortex stack rather than the superconducting transition. Due to additional magnetic screening produced by the second layer each pancake vortex traps a magnetic flux $\Phi_0/2$, i.e., half quantum flux, producing a downwards shift of the stack-evaporation temperature as compared to a bulk system. By means of a renormalisation group analysis we discuss the competition between the vortex-stacks and the pancake vortex unbinding. We determine the $I$-$V$ characteristic and propose an experimental setup which allows to identify the evaporation transition as the resistive transition.

S3Y108 **HTSC-PHOTOSEMICONDUCTOR HYBRID CONTACT STRUCTURES**

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In this paper we report the formation process of "YBa$_2$Cu$_3$O$_{7-x}$ (HTSC ceramic)/BiOHal (semiconducting singlecrystal)" hybrid contact structures(HCS's) and the results of investigation our physical properties. The features of the physical properties "HTSC - photosemiconductor" HCS's become much more significant within the temperature range T<T$_c$, due to the changes in the spectra of elementary excitations of HTSC. The "YBa$_2$Cu$_3$O$_{7-x}$- BiOCl:Ti" and "YBa$_2$Cu$_3$O$_{7-x}$-BiOI "HCSs are heterophotoresistors with large spectral sensitivity (0.31 - 0.80 mkm) and which are suitable for photoelectric analysis of polarisation plane of linearly polarised irradiation.

S3Y109 **Effects of preparation conditions on transport properties of bulk and thin-film MgB$_2$ superconductor**

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Two sets of bulk MgB$_2$ samples were synthesized by annealing in vacuum and in Ar atmosphere. Their resistive critical temperature was found to be in the range 34-39K depending on the preparation conditions. The $\rho$(T) curves were well approximated by the polynomial $\rho_0+\rho_3$T$^m$, where 2.5$\leq$m$\leq$3. The values of $\rho$(T$_c$) differed substantially for various annealing conditions. The quantity of thermoelectric power coefficient S was linear in T at low temperatures and tended to 9-14 $\mu$V/K at room-temperature. Thin films of MgB$_2$ were prepared by PLD on MgO and LaAlO$_3$ substrates. R(T) and S(T) for films were measured and found similar to those of bulk samples.

S3Y110 **Experimental evidence of quantum phase slip phenomena in ultra-narrow superconducting channels**

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A superconducting wire can be considered as quasi-one dimensional if its characteristic transverse dimension is smaller than the coherence length. The shape of the bottom part of the resistive transition R(T) of a not too narrow 1D strip is well described by the model of thermally activated phase slips. However, if the wire width falls into an app.10 nm range, there are predictions that a new phase slip mechanism due to quantum tunneling should be observable. We have developed a method of progressive reduction the transverse dimensions of e-beam lift-off fabricated nanostructures by ion-beam sputtering. The method enables galvanomagnetic measurements of the same sample in between the sessions of etching. Aluminum wires with effective diameter less then 30 nm did show up a low temperature foot at R(T) dependencies, which can be associated with quantum phase slip mechanism.

**S3Y111** **Influence of carbon substitution on the heat transport in single crystalline $MgB_2$**

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We report data on the thermal conductivity $\kappa(T, H)$ and the electrical resistivity $\rho(T, H)$ of single-crystalline superconducting $Mg(B_{1-x}C_x)_2$ ($x = 0.03, 0.06$) in the normal and mixed states at temperatures between 0.6 and 40 K, and in external magnetic fields $H$ up to 50 kOe. The results are analyzed in terms of a combined phononic ($\kappa_{ph}$) and quasiparticle ($\kappa_e$) heat transport and compared with our earlier results on pure $MgB_2$. The substitution of carbon for boron leads to a considerable reduction of the field-induced $\kappa_e$, while $\kappa_{ph}$ seems to be much less sensitive to impurities. The analysis of the $\kappa_e(H)$ data leads to the conclusion that the introduction of carbon enhances mostly the intraband scattering in the $\sigma$-band. While in pure $MgB_2$ the $\sigma$-band is in the pure limit and the $\pi$-band in the dirty limit, carbon doping causes both bands to be in the dirty limit. The interband scattering is rather weak in both cases.

**S3Y112** **Spontaneous Flux Lattice in Ferromagnetic Superconductors**

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A theory is developed for the spontaneous vortex lattice that is expected to occur in the ferromagnetic superconductors $ZrZn_2$, $UGe_2$, and $URhGe$, where the superconductivity is likely of spin-triplet nature. The long-wavelength fluctuations of this spontaneous flux lattice are found to be huge compared to those of a conventional flux lattice, and they are predicted to be the same as those for spin-singlet ferromagnetic superconductors. It is shown that these fluctuations provide a convenient way to observe the spontaneous flux lattice, which would be hard to achieve by other means.

**S3Y113** **Strong-coupling theory of magnetic-exciton-mediated superconductivity in $UPd_2Al_3$**

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There is compelling evidence that the heavy-fermion superconductor $UPd_2Al_3$ can be understood as a dual system of magnetic excitons coupled to delocalised f-electrons. We have computed the superconducting transition temperature $T_c$ and the mass renormalisation $m^*/m_b$ arising from such a dual model (possessing maximal spin anisotropy) using a strong-coupling approach. We find an instability to two possible opposite-spin-pairing states with even- or odd-parity gap functions. Each has a line node perpendicular to the c-direction and total spin component $S_z$=0, in agreement with experiment. The calculated values of $T_c$ and $m^*/m_b$ agree well with experiment for representative values of the coupling constant.

**S3Y114 VORTEX DYNAMICS AT THE RESISTIVE TRANSITION OF THALLIUM AND BISMUTH BASED SUPERCONDUCTORS**

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The temperature dependence of the a.c. resistance of bismuth and thallium based bulk materials as well as of a c-axis oriented single crystal thin films was measured as a function of temperature and magnetic field. Dependence of the resistive superconducting transition and irreversibility field were discussed both in the frame of flux creep model and of the superconducting liquid vortex model. From fitting procedure the experimental data were described very well by the well known exponential formulas. It was concluded that our experimental data can be understood within the formula extracted from the superconducting liquid vortex model with properly fitted parameters.

**S3Y115 Secondary voltage and 3D/2D phase transition in BSrCaCuO single crystals**

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Multicontact configuration is one of the most powerful arrangements for electrical transport measurements applied to study vortex phase transition and vortex phase dimensionality in strongly anisotropic high-$T_c$ superconducting materials. We present electrical transport measurements using a multiterminal configuration, which prove both the existence of guided vortex motion in $Bi_2Sr_2CaCu_2O_8$ single crystals and that secondary voltage in zero external magnetic field is induced by thermally activated vortex loop unbinding. The phase transition between the bound and unbound state of the vortex loops was found to be below the temperature where the phase coherence of the superconducting order parameter extends over the whole volume of the sample. We show experimentally that 3D/2D phase transition in vortex dimensionality is a length-scale-dependent layer decoupling process and takes place simultaneously with the 3D/2D phase transition in superconductivity at the same temperature.

**S3Y116 Paramagnetic limit of superconductors with charge-density waves**

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Superconducting metals with the dielectric gap $\Sigma$ induced by charge-density waves (CDWSs) on nested sections of the Fermi surface (FS) are considered. The paramagnetic limit $H_p$ on the upper critical magnetic field $H_{c2}(T)$ in such substances is calculated. Here $T$ is the temperature. It is shown that due to the similarity between paramagnetic effects in superconductors and metals partially gapped by CDWs, the quantity $H_p$ in CDWSs is always higher than the Clogston-Chandrasekhar value $H_p^{\rm BCS}$. The dependences of $H_p$ on the observed critical superconducting ($T_c$) and CDW ($T_d$) temperatures was obtained for different portions of the nested FS sections. Relevant experimental data for inorganic and organic superconductors with $H_p > H_p^{\rm BCS}$ are analyzed. The conclusion is made that, in a qualitative agreement with the proposed theory, the observation of this inequality may sereve as a hallmark of the electron spectrum CDW instability.

S3Y117 **Effect of Mo and Mn substitution on the crystal structure and thermal properties of $Y_1Ba_2Cu_3O_y$**

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A number of studies have been done on the effect of elemental substitution of yttrium in YBaCuO by various elements of the periodic table. However, little work seems to have been done on the effect of substitution of Y by Mo and Mn on the properties of YBaCuO. The effect of Mo and Mn content on the crystal structure and the coefficient of thermal expansion of $Y_1Ba_2Cu_3O_y$ is investigated in the temperature range 77 to 300K. An increase in the normal state resistivity, a decrease in the transition temperature and a change in structure from orthorhombic to tetragonal are observed with increase in Mo concentration. It is seen that the jump in thermal expansion increases linearly as the Mo concentration is increased. In contrary it is found that there is no structural transformation for Mn substituted compounds. It is observed that the jump in thermal expansion coefficient for Mn doped compounds remains almost constant.

S3Y118 **Superconductivity of semiconducting monochalcogenide two layer heterostructures**

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We report about discovering of superconductivity in two-layer semiconducting monochalcogenide heterostructures PbTe/PbS and PbTe/YbS. The transition temperatures of these heterostructures are in the range 2.6-5.3 K. Comparison of data for such the samples and single monochalcogenide films made it conspicuously clear that superconductivity of the former is connected with interface between two semiconductors. Evidence of low-dimensional nature of interlayer superconducting layer, which follows from measurements of the resistive transitions, critical magnetic fields and magnetoresistivity in a normal state, are obtained.

S3Y119 **Steady phase-slip states in wide superconducting films**

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Resistive current states in wide superconducting tin films with phase slippage have been studied experimentally. These states are characterized by the formation of phase-slip lines (specific Josephson elements) against the background of a dynamic vortex state due to an evolution of the vortex instability in the flux flow. The developed technology of the thermal evaporation allowed fabrication of the tin films with the stable phase-slip states in a relatively wide temperature region due to an optimal specific resistance of the samples and effective heat removal. In this case the thermal instability current is much more than the vortex instability current. A stability of the phase-slip states in respect to the thermal dissipation is discussed. The experimental temperature dependencies of instability currents have been summarized in a form of the diagram model of resistive state (DMRS).

S3Y120 **Low Temperature Structural Study of $Eu_{1+x}(Ba_{1-y}R_y)_{2-x}Cu_3O_{7-d}$ Compounds**

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We report THE FIRST structural study of magnetostriction (MS) in superconductors with rare earth substitutions, corresponding to different concentration of carriers. Connection of volume changes below superconducting transition and MS properties is checked. Neutron and X-ray diffraction studies above and below $T_c$ in magnetic field were performed. They show sufficient difference of unit cell volume in normal and superconducting state. Its field sensitivity testifies the connection of this difference with superconducting transition, which indicates high value of the pressure derivatives of bulk superconducting properties. Its sign in magnetic field shows that volume change at transition sufficiently exceeds thermal contraction contribution.

S3Y121 **Vortex pinning by correlated disorder in nanoparticle doped $MgB_2$**

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Magnetoresistivity and critical current density were measured on five Si-nanoparticle doped ($c \leq 10$ wt.%) and undoped Cu-sheathed $MgB_2$ tapes and wires for temperatures $T \geq 28$ K in magnetic fields $B \leq 0.95$ T. Unlike the irreversibility lines $B_{irr}(T)$ for undoped samples (smooth lines), $B_{irr}(T)$ for doped samples shows a change in slope which is typical for high-temperature superconductors (HTS) with correlated disorder. Microstructural studies of nanoparticle doped $MgB_2$ show uniforlmy dispersed $Mg_2Si$ nanopercipitates which probably act as a correlated disorder ($B_\phi$ is the matching field). But, in contrast to HTS, in nanoparticle doped $MgB_2$ the enhancement of $B_{irr}$ (with respect to undoped one) persists at all field scales (including $B \gg B_\phi$).

S3Y122 **Effect of Pb Content on Magnetic and Transport Properties of Bi(Pb)-2223 Superconducting Ceramics;**

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Superconducting ceramic samples Bi2-xPbxSr2Ca2Cu3O10+d (Bi(Pb)-2223) (x varying from 0 to 1) have been prepared by the standard solid state reaction method. Microstructural properties have been analyzed by means of X-rays Diffraction (XRD) and Scanning Electron Microscopy. Magnetic and transport measurements were used to investigate the superconducting properties of the samples. The transport critical current density shows at 77K a maximum for Pb content between 0.3 and 0.4. The magnetic measurements confirm this behaviour at the same temperature but show a different behaviour at low temperature. Results show that the parameters influencing the critical current density are not only the lead content and the doping level but also the purity of the phase.

**S3Y123 Details of superconducting transition**

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The high resolution measurements of the magnetic flux generated by shielding current induced by applied field in superconducting samples clearly show the distinct mechanism of electron scattering in HTS from that in BCS superconductors. These unique experimental data, with resolution in the order of 1 peV, may be interpreted on basis of elastic and inelastic electron scattering. While the data on Pb is consistent with the BCS model, the data on HTS (YBCO and BSCCO) shows mechanism similar to that in La, which is regarded as the type-I superconductor but not well consistent with the BCS. Fermi surface nesting, electron-lattice instability, and displacive structural transition with modulated phases are characteristic for La. This new experimental data and its interpretation should be relevant for understanding of correlated (paired) electrons in HTS.

Z. Janu et al., Europhys. Lett 64 (2003) 399.

**S3Y124 Quantum Hall effects in layered disordered superconductors**

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Layered singlet paired superconductors with disorder and broken time reversal symmetry are studied. The phase diagram demonstrates charge-spin separation in transport. In terms of the average intergrain transmission and the interlayer tunnelling we find quantum Hall phases with spin Hall coefficients of $\sigma_{xy}^{spin} = 0, 2$ separated by a spin metal phase. We identify a spin metal-insulator localization exponent as well as a spin conductivity exponent of $\approx 0.9$. In presence of a Zeeman term an additional $\sigma_{xy}^{spin} = 1$ phase appears.

**S3Y125 Some features of the spin fluctuation Cooper-pairing scenario in layered cuprates: kink and resonance peak**

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In our studies we have calculated self-consistently the pronounced momentum and frequency dependence of the self-energy originating from scattering of the quasiparticles on spin fluctuations within a unified theory for Cooper-pairing in hole-doped high-Tc cuprates[1]. We find that this coupling results in a kink structure in the dispersion $\omega(k)$ which agrees well with recent ARPES experiments. Furthermore, using a two-dimensional Hubbard Hamiltonian we find that the resonance peak in the magnetic susceptibility, appears only in the superconducting state and it scales with $T_c$.

[1] D. Manske, I. Eremin, and K.H. Bennemann, Phys. Rev. Lett. 87, 177005 (2001); Phys. Rev. B 67, 134520 (2003).

**S3Y126** **STRUCTURE AND PHYSICAL PROPERTIES OF THE HALOGEN-DOPED BISMUTH- 2234 HIGH-TEMPERATURE SUPERCONDUCTORS**

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We report the results of preparation, X-ray structure and magnetic properties of $Bi_{1.6}Pb_{0.4}Sr_2Ca_3Cu_4O_{12-z}Hal_z$ (Hal=F,I) high $T_c$-superconductor and effect of oxygen-halogen substitution. The $Bi_{1.6}Pb_{0.4}Sr_2Ca_3Cu_4O_{12-z}Hal_z$ samples (Hal=F,I) with z=0.0-1.0 were prepared by many steps solid state reaction method. The external magnetic field with magnitude H>2.5 T leads to radical changes of magnetic properties iodine doped Bi-2234 HTSC. After first AFM- transition at $T_N$ = 67.8 K the samples undergoes superconducting(SC-) transition with $T_c$ ~62K. The AFM- and SC- states coexist in 15K - 62K temperature range, 2.5T - 4.5T external magnetic field range and iodine concentration ranges z=0.075-1.0. The shape of the ferromagnetically ordering at $T_c$= 14.625 K depends on the way of temperature cycling and have irreversibility character.

**S3Y127** **Heat capacity of superconductors with charge-density waves**

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Self-consistent equations for temperature-, $T$, dependent superconducting, $\Delta$, and dielectric, $\Sigma$, order parameters are solved in the partial-dielectrization model of Bilbro and McMillan for superconductors with charge-density waves (CDWs). It has been shown that for the close enough structural , $T_d$, and superconducting , $T_c$, phase transition temperatures,with $T_d > T_c$, $\Delta(T < T_c)$ can exceed $\Sigma(T)$. The discontinuity $\Delta C$ at $T = T_c$ of the electronic heat capacity $C(T)$ has been shown to be always smaller than the Bardeen-Cooper-Schrieffer value. The effect is detectable in a wide range of the model parameters. Experimental implications for CDW superconductors, such as A15 compounds and high-$T_c$ cuprates are suggested and discussed.

**S3Y128** **Normal and mixed state Hall effect in $(Hg_{0.9}Re_{0.1})Ba_2CaCu_2O_{6+\delta}$ fully textured HTS's thin films**

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Temperature and magnetic field dependence of the Hall effect in the normal and mixed state of fully textured HgRe-1212 HTS's thin films prepared by laser ablation deposition have been studied. The longitudinal resistivity ($\rho_{xx}$) and Hall resistivity ($\rho_{xy}$) were measured for a wide range of magnetic fields from 125 mT to 12 T with the field perpendicular to the ab plane and the current in the ab plane. A sign change of the Hall resistivity is observed in fields below 3 T in the region close to $T_c$. The temperature dependencies $\rho_{xx} \propto T$ and $\rho_{xy} \propto 1/T$ have been observed for HgRe-1212 thin film. Anderson's formula, namely, $\cot \theta_H = \alpha T^2 + \beta$ remains valid for temperatures $T$ between $T_c$ and 200 K. In the region approaching the zero resistance state or in the mixed state a power-law behavior is observed, where $\rho_{xy}$ scales to a power-law function of $\rho_{xx}$: $\rho_{xy} = A\rho_{xx}^\beta$, $\beta$ with increasing from 1.02±0.044 to 1.68±0.0087 as the field increases from 1 to 12 T.

**S3Y129** **Zeeman splitting in multiple-band superconductors**

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We present a study of Zeeman splitting effects in multiple-band superconductors. It is shown that a two-band superconductor displays several free energy local minima at low temperature leading to an enriched phase diagram. In particular, at low temperature a first-order transition occurs between two superconducting phases. A cascade of first-order transitions occurs in the n-band case.

**S3Y130** **Vortex lattice in tilted magnetic fields in Mo/Si superconducting multilayers**

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We report experimental results of the vortex lattice structure investigation in Mo/Si superconducting multilayers. Resistivity and critical current measurements in a parallel and in a wide range of tilted magnetic fields have been performed. The non-monotonic dependence of the $R$ vs $H$ and $I_c$ vs $H$ observed indicates the existence of commensurate vortex lattice states in parallel magnetic fields. In a range of small field inclination ($\theta < 2.5°$) the lock-in state exists. At larger field inclinations, in a range $6 - 30°$, non-monotonic $R$ vs $H$ dependencies testifying about commensurability effect reappear again. It may be considered as evidence of crossing vortex lattice formation. The phase diagram magnetic field-angle for different vortex lattice states is obtained.

**S3Y131** **Effect of pulse RF magnetic field on HTSC powders**

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The sample of HTSC powder in the constant magnetic field $B_0$ at temperature $T < T_c$ was irradiated by pulses of RF magnetic field $B_\sim$. The stable echo-signals $U_{echo}$ following an RF multipulse sequence have been observed. The experimental data $U_{echo}$(T,$B_0$,$B_\sim$,etc.) are discussed in terms of stimulated fluxoid oscillations which excite, in its turn, an ultrasonic wave. The long-lived echo phenomenon (proposed for application in quantum computer memory) is determined by conservation of fluxoid oscillations in the form of a standing wave when there is no interchange of energy between fluxoids and lattice. Quantitative description of the experiments is done using the model of localized electron pairs, where superconducting properties are determined by charge transport along a band formed by pairs of carriers (bosons) belonging to $U^-$-centers. The model is best suited to describe some observed pequliarities like clear maximum in the dependence $U_{echo}(B_0)$.

**S3Y132** **Excitation of Spin Waves in Superconducting Ferromagnets**

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Excitation of spin waves in a superconducting ferromagnetic slab is analyzed theoretically. We calculated the surface impedance for various orientations of the ferromagnetic spontaneous magnetization with respect to the sample surface. Dissipation due to normal currents is taken into account. We found and studied the impedance singularities related to threshold frequencies for spin wave excitation. With a suitable choice of parameters, a regime is possible, in which an electromagnetic wave excites in the material two propagating spin waves, one of which has a negative group velocity. Implications of our results for unconventional superconductors with broken time reversal symmetry are discussed. The analysis demonstrates that the experimental investigation of spin wave modes can be an effective probe of unusual magnetic properties of superconducting ferromagnets.

S3Y133 **Oxygen superstructures throughout the phase diagram of** $(Y, Ca)Ba_2Cu_3O_{6+x}$

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Short-range lattice superstructures have been studied with high-energy x-ray diffuse scattering in underdoped, optimally doped, and overdoped $(Y, Ca)Ba_2Cu_3O_{6+x}$. A new four-unit-cell superstructure was observed in compounds with $x \sim 0.95$. Its temperature, doping, and material dependence was used to attribute its origin to short-range oxygen vacancy ordering, rather than electronic instabilities in the $CuO_2$ layers. No significant diffuse scattering is observed in $YBa_2Cu_4O_8$. The oxygen superstructures must be taken into account when interpreting spectral anomalies in $(Y, Ca)Ba_2Cu_3O_{6+x}$.

S3Y134 **Nucleation of superconductivity and vortex matter in superconducting microstructures**

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We study the evolution of the superconducting state in a perforated disk by varying the size of the hole. The superconducting properties are investigated by means of transport measurements around the superconducting/normal phase boundary $T_c(H)$. The effect of breaking the axial symmetry of the structure by moving the hole away from the center of the disk is also studied. A transition from a one-dimensional to a two-dimensional regime is seen when increasing the magnetic field for disks with small holes. Hall magnetometry measurements were performed on a superconducting mesoscopic square and triangle. The stability of some vortex patterns imposed by the sample geometry is discussed. This work has been supported by the IWT-Vlaanderen, the Belgian IUAP, the Flemish FWO, the Research Fund K.U.Leuven GOA/2004/02 and by the ESF VORTEX programmes.

S3Y135 **Characteristic features of differential conductivity of transparent superconducting structures with non-uniform transparency of the tunnel barrier.**

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By means of Bogolyubov - de Gennus equations solution in approximation of homogeneous superconductors in the framework of Blonder-Tinkham-Klapwijk (BTK) approach the computer modeling of current transport in superconducting NbN-I-Pb tunnel junctions for a case of non-uniform thickness of the tunnel barriers is carried out. It is established, that computer modeling by the given method allows by the account of Andreev reflection of quasiparticles to restore probabilities distribution function of occurrence in transition of tunnel barrier sites with a various transparency. Key words: differential conductivity, tunnel junctions, barrier transparency, Bogolyubov-de Gennes equations, quasiparticle current.

S3Y136 **Spontaneous Magnetic Flux Generated by a Superconducting $\pi$-Loop**

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We have fabricated Nb-loops containing a ferromagnetic Josephson junction based on a dilute PdNi-alloy. For proper values of the ferromagnetic layer thickness and exchange field, $\pi$ coupling can be realized. By varying the applied magnetic field, the phase difference across the weak link is tuned. The magnetic response of the loops has been measured using a micron-sized hall sensor. When comparing the loops with and without $\pi$-junction, the $\pi$-loop displays asymmetric switching behavior with respect to the applied flux. When cooling down the loop below $T_c$ in zero applied field, a spontaneous current is detected which provides *half*-integer flux quantization in the $\pi$-loop.

S3Y137 **Role of zinc and calcium in the normal-state band spectrum modification of co-doped $YBa_2Cu_3O_y$**

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The results on $T_c$ and the thermopower for three series of the $Y_{1-x}Ca_xBa_2Cu_{3-x}Zn_xO_y$ ($x$=0.0-0.25) samples with different oxygen content are presented. For all the series the $T_c$ value is observed to change in a different way for $x < 0.1$ and $x > 0.1$. An analysis of the data within a narrow-band model allows determining the main band spectrum parameters and tracing their variation with $x$. The effective bandwidth is shown to have a tendency to decrease, whereas the band filling and band asymmetry degrees remain almost unchanged with doping. The roles of zinc and calcium in $T_c$ variation, $S(T)$ modification, and conduction band transformation are discussed. It is concluded that a band reconstruction is caused by two opposite reasons, i.e., introducing states into upper band half due to the calcium effect and a states transfer from the band due to the zinc effect.

S3Y138 **Frequency domain response in networks of multimode waveguides**

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The interface response theory [1] will be applied to systems of multimode waveguides with special boundary conditions at the waveguides junctions. Expressions for the frequency domain Green functions will be given for hydraulic networks with elastic tubes and for their electric counterparts: coupled transmission lines. The simplest case of axially symmetric modes, the flow dominated mode and the elasticity dominated one, will be treated in most detail. Examples of modeling pulse waves transmission and reflection in arterial system will be presented. The role of nonlinear elements will be discussed [2]. Application to transport properties in multimode nanosystems will be mentioned.
[1]. L. Dobrzynski, Surf. Sci. Reps. **11**, 139 (1990) [2]. P. Zieliński, A. Kułak, L. Dobrzynski and B. Djafari-Rouhani, Eur. Phys. J. B **32**, 73 (2003)

## S3Y139 **Dipoles and Ion Channels**

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The study of the transport in ion channels is complicated by the presence of the protein walls, whose interaction with ions is not well understood [1,2]. In this paper we analyse the effect of ion current on the dipoles which are in the protein wall of biological ion channels. Ion current determines an orientation of the dipoles. In a special conditions this orientation causes an increases of ion average drift velocity and we have calculated the new ion current. Some effects of current increase are presented in the last section.  References [1]S.Kuyucak, M.Hoyles, S.H.Chung,Biophys.J.,74,1,22,(1998). [2]D.G.Levitt, J.Gen.Physiol.,113,6,789,(1999).

## S3Y140 **Magnetization Studies of the Rubredoxin and Desulforedoxin from** *D. gigas*

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The *Desulfovibrio gigas* rubredoxin and desulforedoxin are nonheme iron proteins. Both metalloproteins contain a single $Fe(S-Cys)_4$ center in a high spin configuration (S=5/2), in the oxidised form, that is converted to a S=2 in the reduced form. In rubredoxin the iron-sulfur center presents a tetrahedral geometry while in desulforedoxin it has a distorted tetrahedral geometry. Their multifield magnetizations were measured as a function of temperature for the oxidized and reduced states. Data were analyzed on the base of the spin-Hamiltonian, yielding the values of the zero field splitting parameters D and E/D. These are reported and compared to other techniques' results. (Support: FCT, POCTI, co-financed by FEDER (POCTI/35324/FIS/2000))

## S3Y141 **Magnetization Studies of split-Soret cyt. *c* from *D. d.* ATCC 27774**

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Split-Soret cytochrome *c*, isolated from the facultative sulfate/nitrate reducing bacterium *Desulfovibrio desulfuricans* ATCC 27774, is a novel type of metalloprotein containing two *c* type heme and a [2Fe-2S] core [1]. We report magnetization measurements on oxidized and different reduced states up to 5.5 T and from 2 to 200 K. Experimental conditions were first validated with monohemic $c_{552}$ cyt. in oxidized (neutral and acidic pH) and reduced states; magnetization curves, analysed with the spin-Hamiltonian model, yielded the expected S values. The magnetization data for split-Soret were analysed and spin concentrations and zero field splitting parameters were obtained and are discussed based upon previous EPR results. [1] C. Costa et al., J. Inorg. Chem. (1997) 67, A09. (Support: FCT, POCTI, co-financed by FEDER (POCTI/35324/FIS/2000))

## S3Y142 **COOPERATIVITY OF FOLDING TRANSITION IN MODEL PROTEINS**

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The thermodynamic cooperativity of the temperature-driven transition between folded and unfolded states of two-state proteins is studied using off-lattice Go models. By the Langevin dynamics simulations it was shown that the sharpness of the transition depends on the viscosity of environment. Such a dependence was found to be stronger for sequences which contain more beta sheets compared to helix-based sequences. The scaling of cooperativity of off-lattice models is governed by the same scaling exponent obtained for their lattice counterparts and it coincides with the experimental result.

S3Y144 **Controlling the elastic properties of polyelectrolyte multilayers**

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Polyelectrolyte multilayers consisting of poly(diallyldimethylammonium chloride) (PDADMA) and poly(sodium-4-styrenesulfonate) (PSS) were studied with a quartz crystal microbalance (QCM) utilizing a novel method to determine the elastic properties of the films. The multilayer films were made thick enough to reveal the elastic properties of the bulk material of the film. Several hundreds of layers were deposited using a fully automated multilayer deposition machine. We found out that in addition to the increase in the bilayer mass, a remarkable increase of stiffness of the polyelectrolyte multilayer was observed while altering the counteranion used in the deposition process. The increase of stiffness was found to be nearly comparable to the glass transition of common polymers. The correlation of storage shear modulus and mass density to the hydration entropy of the anion could be clearly observed.

S3Y148 **The phase transition of liquid phosphorus by ab-initio calculation**

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We have carried out ab initio molecular-dynamis simulations for liquid phosphorus under high temperature and high pressure in order to investigate the microscopic mechanism of the recently observed liquidliquid phase transition of liquid phosphorus. We have shown that the structural phase transition corresponds to the structural change from the molecular liquid composed of stable tetrahedral P4 molecules to the polymeric liquid with complex network structure. It is also found from our calculated electronic structure that this structural change gives rise to the nonmetalmetal transition, which is the transition from the nonmetallic molecular liquid to the metallic polymeric liquid. In addition, we report the dynamic properties such as the velocity autocorrelation functions, intermediate scattering functions and the dynamic structure factors.

S3Z201 **Smeared phase transition in a three-dimensional Ising model with planar defects: Monte-Carlo simulations**

Rastko Sknepnek[1], Thomas Vojta[1]
*1) University of Missouri – Rolla*

We present results of large-scale Monte-Carlo simulations for a three-dimensional Ising model with short-range interactions and planar defects, i.e., disorder perfectly correlated in two dimensions. We show that the phase transition in this system is smeared, i.e., there is no single critical temperature, but different parts of the system order at different temperatures. This is caused by effects similar to but stronger than Griffiths phenomena. In an infinite-size sample there is an exponentially small but finite probability to find an arbitrary large region devoid of impurities. Such a rare region can develop true long-range order while the bulk system is still in the disordered phase. We compute the thermodynamic magnetization and its finite-size effects, the local magnetization, and the probability distribution of the ordering temperatures for different samples. Our Monte-Carlo results are in good agreement with a recent theory based on extremal statistics.

**S3Z202** **Mixed Spin Effects on the Commensurate Phases of the Ising Model with Anisotropic Competing Interactions**

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By molecular-field (MF) approximation and Monte Carlo (MC) simulation, we analyzed the $mixed$-$spin$ axial next-nearest-neighbor Ising model, which is composed of alternately stacked $S$ ($= \pm 1, 0$) and $\mu$ ($= \pm 1/2$) ferromagnetic layers with competing interlayer interactions along $c$-axis. The MF calculations predicted the appearance of the spatially modulated partially disordered phases (PDPs) having layer-magnetization along $c$-axis $\uparrow \circ \downarrow \circ$ and $\bullet \uparrow \bullet \downarrow$ ($\circ$ and $\bullet$ denote paramagnetic $\mu$- and $S$-layer, respectively.) and the crossover phenomenon between these two PDPs. MC results of layer-magnetizations, their lattice-size dependences and spin-correlations are qualitatively consistent with ones suggested by MF theory.

**S3Z203** **Riemann-Silberstein representation of the complete Maxwell equations set**

M.V. Cheremisin[1]
*1) A.F.Ioffe Physical-Technical Institute, St.Petersburg, Russia*

Complete set of Maxwell equations is represented [1] by single equation using the Riemann-Silberstein vector[2] $\mathbf{F} = \mathbf{E} + i\mathbf{B}$. We demonstrate that the Fourier form of invariants $E^2 - B^2$ and $\mathbf{EB}$ is proportional to dissipated power and equal to zero respectively. [1] M.V.Cheremisin, hep-th/0310036 [2] L.Silberstein, Ann. de Phys.(Leipzig),22, 579, ibid 24, 783,1907

**S3Z204** **Exotic vs. conventional scaling and universality in a disordered bilayer quantum Heisenberg antiferromagnet**

Rastko Sknepnek[1], Thomas Vojta[1], Matthias Vojta[2]
*1) Department of Physics, University of Missouri –Rolla*
*2) Institut für Theorie der Kondensierten Materie, Universität Karlsruhe*

We present large-scale Monte-Carlo simulations of a two-dimensional bilayer quantum Heisenberg antiferromagnet with random dimer dilution. In contrast to the exotic scaling scenarios found in many other random quantum systems, the quantum phase transition in this system is characterized by a finite-disorder fixed point with power-law scaling. After accounting for strong corrections to scaling, characterized by a leading irrelevant exponent of $\omega \approx 0.48$, we find universal, i.e., disorder-independent, critical exponents $z = 1.310(6)$ and $\nu = 1.16(3)$. We discuss the consequences of these findings and suggest new experiments.

**S3Z205** **Absence of diffusion in high-dimensional random lattices**

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*1) Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, CZ-18221 Praha 8, Czech Republic*

A model of noninteracting disordered electrons is studied in high spatial dimensions in order to develop a mean-field description of Anderson localization transition. Off-diagonal one- and two-particle propagators are found to behave as Gaussian random variables with respect to momentum summations. With this simplification the parquet equations for two-particle irreducible vertices are reduced to an algebraic equation for a single local quantity. The time-reversal invariance, displayed as the electron-hole symmetry of two-particle functions, plays a substantial role in such a reduction as well. We find a disorder-driven bifurcation point in the resulting equation that signals vanishing of diffusion and onset of Anderson localization. There is no bifurcation in dimensions $d = 1, 2$ where all states are localized. A natural order parameter for Anderson localization pops up in the course of the construction.

**S3Z206** **Simple model of phononic crystal vibrations**

Arnold M. Kosevich[1], Oleksandr V. Kotlyar[1]

*1) B.Verkin Institute for Low Temperature Physics and Engineering of the National Academy of Sciences of Ukraine*

Propagation of elastic waves in a phononic crystal composed of infinite plane-parallel layers of two alternating substances is studied. The wave vector is inclined at arbitrary angle with respect to the normal to the layers. A special case is discussed when both the thickness l and elastic module G of one material tend to zero under the condition that the ratio G/l to be a constant. The superlattice of such a type is equivalent to a structure constructed of single material layers with the special boundary conditions at the junctions supposing the continuity of normal strains and the jump of displacements. The dispersion relations for waves with longitudinal and longitudinal-transversal polarization are derived. It is shown that the band structure is characterized in both cases by band gaps growing with frequency. The dependence on the wave vector inclination and limited transverse size of the superlattice is studied.

**S3Z207** **STATISTICAL THEORY OF ORIGIN OF INTRINSIC CURRENT CARRIERS IN SEMICONDUCTORS**

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Well known, fluctuations of phonon local concentration in crystal leads to creation of free electrons and holes in semiconductors at $kT << E_g$. Unfortunately, in the literature there are no publications, devoted to analysis of this process.

In the presented work theory of origin of free current carrier in semiconductors related with fluctuations of local phonon concentration is developed. It was supposed that fluctuations of phonon local concentration arises in reasonably small excited area contained $\alpha$ lattice sites. Probability of this fluctuations in excited area of semiconductor was calculated by Poison formula.

The volume of excited area is evaluated : for silicon and germanium the excited area contains $\alpha \sim$ 11 - 12 lattice sites and in the case of GaAs - $\alpha \sim$ 13- 14.

**S3Z208** **Critical Dynamics: theory for time-dependent intensity correlations measured by X-ray microdiffraction**

Klaus Mecke[1], C. Mocuta[2], H. Reichert[1]

*1) MPI für Metallforschung, D-70569 Stuttgart, Germany*
*2) ESRF, F-38043 Grenoble, France*

We studied the dynamics of critical fluctuations in $Fe_3Al$, which exhibits an order-disorder phase transition. One can measure pronounced effects on the time-course of the intensity of a superstructure peak if the beam is well focused and probe only a sub-micron sized sample. Starting from a stochastic Langevin equation for a non-conserved order-parameter the four-point structure function can be calculated and directly related to the measured time-dependent intensity-intensity correlation function with the correlation time $\tau$ as only free fit parameter. We find a strong dependence on temperature, e.g. an increase of $\tau$ close to the critical point. The agreement of theory and experiments for various spatial and time resolutions demonstrate the potential of partially coherent x-ray microbeams for the direct observation of fluctuation phenomena at critical phase transition.

**S3Z209** **NON-MAXWELL CHARGE RELAXATION: MECHANISMS AND NEW NONEXPONENTIAL LAWS**

A. Bainova[1], V. Arkhincheev[2]

*1) Buryat State University, Russia*
*2) Department for physical problems Buryat Science Center of SB RAS, Russia*

**S3Z210** **Energy flow density of a quasiparticle of a continuous medium with arbitrary energy-momentum relation**

I.N. Adamenko[1], K.E. Nemchenko[1], I.V. Tanatarov[1]
*1) V.N. Karazin Kharkov National University*

In this work we consider the density of energy flow of a quasiparticle in a continuous medium with arbitrary energy-momentum relation $\omega(k)$. The deviation of the relation $\omega(k)$ from linearity always appears when the interaction between not only the adjacent physically infinitesimal peaces of matter is taken into account. So we use the model of continuous medium, in which the relation between the variables of continuous medium is non-local. Starting from the Hamiltonian, we obtain a general expression for the density of energy flow. For a wave packet a simple relation is derived for this quantity, which generalizes the ordinary form of it to the case of arbitrary $\omega(k)$.

There are $R^-$ rotons in superfluid helium and phonons in solids, that have negative group velocity, $d\omega/dk < 0$. It can be seen from this work that the density of energy flow of such a quasiparticle must be oppositely directed to its momentum.

**S3Z211** **Peculiarities of Critical Opalescence Spectrum in Liquids with Reduced Geometry**

K.A. Chalyy[1], L.A. Bulavin[1], A.V. Chalyi[2]
*1) Faculty of Physics, Kiev Taras Shevchenko National University, Ukraine*
*2) Department of Biophysics, National Medical University, Ukraine*

The specific features of light critical opalescence for one-component finite-size liquid systems with geometry of cylinder and plane layer are investigated. The modified dynamical scaling hypothesis, which describes the non-equilibrium physical properties (in particular, features of critical opalescence spectrum) for the spatially limited near-critical liquid, is formulated. The dependence of width $\Gamma_c$ of the central component of Rayleigh line is obtained for the liquid in a small cylindrical volume. It is shown that the reduction of characteristic size of the system (for chosen geometry — the radius of a cylinder) leads to increasing of width $\Gamma_c$ of the central component. Moreover, the integrated intensity of light scattering remains finite at the bulk critical temperature while it demonstrate significant growth at the new critical temperature of a system with reduced geometry.

**S3Z212** **The role of short-range interactions in one-dimensional proton conductor**

Ihor Stasyuk[1], Oleg Vorobyov[1]
*1) Institute for Condensed Matter Physics, Lviv, Sventsitskii 1 str., Ukraine*

Discovery of superionic conductors has raised considerable interest to the systems where conductivity is caused by the proton transport. Although there are many microscopic processes that act in proton subsystem its investigation is very important.

We consider the fermionic model of one-dimensional proton conductor, which takes into account the proton transfer in the spirit of two-stage Grotthuss mechanism and the interactions between nearest protons. These short-range interactions are considerably strong thus we take them into account in the zero-order Hamiltonian.

We calculate the proton energy spectrum and investigate the chemical potential behaviour at different proton concentrations. The spectrum consists of the several bands and depending on the average concentration of protons the system can be in either quasi-metallic or insulating state.

**S3Z213** **The generalization of Dykhne-Keller theorem for effective conductivity of random medium for a rhomb case.**

V. Arkhincheev[1]
*1) Department for physical problems of Buryat Science Center, SB RAS, Russia*

**S3Z214** **Mean-field theory of spin glasses: Replicated TAP free energy and its thermodynamic homogeneity.**

Lenka Zdeborova[1], Vaclav Janis[1]
*1) Institute of Physics AS CR, Prague, Czech Republic*

We study the Sherrington-Kirkpatrick model using a recently introduced technique called the "real replica" method. We can avoid within this scheme the replica trick and the Parisi ansatz on the replica symmetry breaking. With a small interaction between real replicas, breaking their independence, we derive a TAP-like free energy with new order parameters. They are overlap susceptibilities, i. e., the response on the replica-independence breaking interaction. We then average this replicated TAP free energy over all configurations of spin-spin interactions. The Euler condition of homogeneity of the free energy demands independence of the final result on the number of real replicas. With this in mind we study saddle-point equations first for integer then for real numbers of replicas. From explicit calculations we deduce symmetries of the order parameters. The result is formally equivalent to the Parisi discrete full step replica symmetry breaking scheme.

**S3Z215** **Non-equilibrium Relaxation MC Study on the Phase Transition into the Partially Disordered State in the ANNNI Model**

Y Muraoka[1], T Kasama[2], H Nishiyama[1], T Idogaki[2]
*1) Dept. of Gen. Edu., Ariake Natl. Coll. of Tech., Omuta, Fukuoka 836-8585, Japan*
*2) Dept. of Applied Quantum Physics, Kyushu Univ., Fukuoka 812-8581, Japan*

We consider the 3D ANNNI model, which is composed of two kinds of alternately stacked ferromagnetic layers with different intralayer interactions. In this model, there exist the partially disordered states(PDS). In the phase transition from the ground state to the $k=1/4$ PDS, to estimate the critical temperature and the exponent, the Monte Carlo simulation is performed using the Non-equilibrium relaxation on simple cubic lattice. The order parameter in ground state and the sublattice magnetization rapidly relax toward values in the equilibrium state near the critical point. We discuss the possibility of the weak universality.

**S3Z216** **Ab initio spectra of the low-pressure phases of zirconia**

L.K. Dash[1], N. Vast[1], P. Baranek[1], M.C. Cheynet[2], L. Reining[1]
*1) LSI, Ecole Polytechnique, 91128 Palaiseau, France*
*2) LTPCM/ENSEEG/CNRS, 38402 Saint-Martin d'Heres, France*

Zirconia ($ZrO_2$) is of current technological interest due to its high strength, excellent dielectric properties, and stability under irradiation. Using ab initio techniques, we study the low-pressure phases of $ZrO_2$, in which the coordination of the Zr atom varies from 7 in the monoclinic phase, to 8 in the tetragonal and cubic phases, and 6 in the hypothetical rutile phase. We calculate spectra and compare them to experimental spectra from various techniques (photoemission, BIS, EELS and Raman spectroscopy) to directly relate the features of the spectra with the electronic structure of each phase. We have calculated the ground state properties using density functional theory (DFT) and use time-dependent DFT to calculate the dielectric function. We discuss the effect of the local coordination on each type of spectra and find our theoretical results in good agreement with experimental data.

**S3Z217** **Cylindrically Confined Helium Heat Capacity: Theory Verification**

K.A. Chalyy[1]

*1) Faculty of Physics, Kiev Taras Shevchenko National University, Ukraine*

The validity of the proposed theoretical approach to finite-size effect on liquid helium heat capacity in the close vicinity of $\lambda$-transition temperature $T_\lambda$ is verified by comparing it with high-resolution experimental data. The expression for the heat capacity keeps special parameters, which are related to the cylindrical form of the system. Actual analytical calculation are conducted without taking into account the gravity effect. It makes possible an easy comparison with the data of correspondent experiments. It is shown that the theoretical approach to the problem of finite-size effect gives the results that are reasonably match to experimental data over the wide range of system's sizes from tens of nanometers up to few micrometers for the cylindrical type of confinement geometry. The dependencies of the shift of transition temperature on the cylinder size and boundary conditions are analyzed. The agreement of the results with the predictions of finite-size scaling theory is confirmed.

**S3Z218** **Inelastic electron transport in metallic atomic wires**

T. Frederiksen[1], M. Brandbyge[1], N. Lorente[2], A.-P. Jauho[1]

*1) Department of Micro and Nanotechnology, Technical University of Denmark, Oersteds Plads, Bldg. 345E, DK-2800 Lyngby, Denmark*

*2) Laboratorie Collisions, Agregats, Reactivite, IRSAMC, Universite Paul Sabatier, 118 Route de Narbonne, F-31062 Toulouse, France*

We describe a method for calculating dc current-voltage characteristics of nanostructures connected between metallic leads taking into account electron-vibration scattering inside the device. The method is based on nonequilibrium Green's functions and a treatment of the electron-vibration interaction in the self-consistent Born approximation. In particular we study transport through atomic Au wires. With a simple tight-binding model as well as with full ab initio methods we determine the normal modes of vibration, the electron-vibration couplings, and the influence of the different modes on the conductance. We find that inelastic scattering gives rise to one characteristic drop in conductance beyond a threshold voltage.

**S3Z219** **The critical behaviour of the mean spherical model in the presence of three external fields**

Magdy Amin[1]

*1)*

 Explicit expressions are derived for the free energy, and the magnetization profile of the three-dimensional mean spherical model with a layer geometry of finite thickness L, under Neumann-Dirichlet boundary conditions in the presence of three external fields: a bulk field, a step-like (+ -) field, and a surface field acting on the l-th layer. The scaling functions that govern the critical behaviour of the system are derived and, with the use of the asymptotic properties of these functions, various predictions of the Privman-Fisher scaling hypothesis are verified in the finite-size scaling regime.

**S3Z220** **Quantum instanton calculation of isotopic effects on reaction rate constants**

Jiri Vanicek[1], W.H. Miller[1]
*1) Pitzer Center for Theoretical Chemistry, U. of California, Berkeley*

We present a general quantum-mechanical method suitable for numerical evaluation of the isotopic effects on the rate constants of chemical reactions. Our method is based on the quantum instanton approximation [1-3] and on the Metropolis Monte-Carlo path integral evaluation of the Boltzmann operator matrix elements. The method is more accurate than existing transition-state theory or semiclassical instanton method since we do not assume a single reaction path and do not use a semiclassical approximation of the Boltzmann operator. In order to calculate the isotopic effect we use a "charging algorithm," whereby the mass of the isotope is continuously changed from the initial to the final value. Direct calculation of the isotopic ratio turns out to be much more efficient than finding the absolute rate constants first and then calculating their ratio. While the Monte-Carlo implementation should make the method accessible to systems with a larger number of atoms, we present numerical results for the Eckart barrier and for the reactions $H + H_2 \rightarrow H_2 + H$ and $H + DH \rightarrow HD + H$.

[1] W.H. Miller, Y. Zhao, M. Ceotto, and Sandy Yang, J. Chem. Phys. **119**, 1329 (2003).
[2] T. Yamamoto and W.H. Miller, J. Chem. Phys. (in press).
[3] Y. Zhao, T. Yamamoto, and W.H. Miller, J. Chem. Phys. (in press).

**S3Z221** **The phase transition of liquid phosphorus by ab-initio calculation**

Yasuhiro Senda[1], Fuyuki Shimojo[2], Kozo Hoshino[3]
*1) Department of Computational science, Kanazawa University*
*2) Faculty of Integrated Art and Science, Hiroshima University*
*3) Department of Physics, Kumamoto University*

We have carried out ab initio molecular-dynamis simulations for liquid phosphorus under high temperature and high pressure in order to investigate the microscopic mechanism of the recently observed liquidliquid phase transition of liquid phosphorus. We have shown that the structural phase transition corresponds to the structural change from the molecular liquid composed of stable tetrahedral P4 molecules to the polymeric liquid with complex network structure. It is also found from our calculated electronic structure that this structural change gives rise to the nonmetalmetal transition, which is the transition from the nonmetallic molecular liquid to the metallic polymeric liquid. In addition, we report the dynamic properties such as the velocity autocorrelation functions, intermediate scattering functions and the dynamic structure factors.

# Focused Sessions 8:30 – 10:00

*Plasmonics with metal nanoparticles* **Room B**

F4B1 **Metal nanoparticles as versatile nanotools: From optoelectronics to biophotonics**

Thomas A. Klar[1]

*1) Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Germany*

Noble metal nanoparticles show a pronounced optical resonance in the visible range of the electromagnetic spectrum, the so called nanoparticle plasmon resonance. This resonance manifests itself in the scattering as well as in the absorption spectrum.

Metal nanoparticles interact strongly with their immediate nanoenvironment: Nanoparticles absorb energy from surface bound fluorescent molecules but also change their radiative lifetime [1]. Hence, fluorophore/gold-nanoparticle composite systems are promising resonant energy transfer pairs. Furthermore, a change in the refractive index of the surrounding shifts the scattering spectrum of the nanoparticles. These effects open up ways to novel and fascinating applications in optoelectronics [2] and biophotonics [3].

[1] Phys. Rev. Lett. 89, 203002 (2002)[2] Appl. Phys. Lett. 81, 171 (2002)[3] Nano Letters, 7, 937 (2003)

F4B2 **Nano-components for plasmonics**

J.R. Krenn[1]

*1) Institute for Experimental Physics and Erwin Schroedinger Institute for Nanoscale Research, Karl-Franzens-University Graz, Austria, WWW: nanooptics.uni-graz.at*

Recent advances in nanoscale fabrication and imaging techniques have contributed significantly to the insight in optical effects based on surface plasmons (SPs). These mixed photon-electron excitations at metal surfaces are of specific interest due to their nanoscale sized optical fields, a strong field enhancement and a temporal response on the sub-10 fs time scale. I will give an overview of recent results on SP optics based on nanostructured metal surfaces with an emphasis on metal nanoparticles. These results include two-dimensional optical devices, non-diffraction limited SP waveguides and single nanoparticles or regular arrays thereof, for which a precise tuning of the local field enhancement and SP lifetime was achieved. The latter point includes surface enhanced molecular spectroscopy.

F4B3 **Microscopy, spectroscopy and manipulation of single gold clusters**

Vahid Sandoghdar[1]

*1) Laboratory of Physical Chemistry, Swiss Federal Institute of Technology (ETH)*

Optical properties of metallic nanoparticles have fascinated scientists for several centuries. In particluar there has been a recent revival of interest in these systems from the fabrication point of view as well as theoretical modelling. In the past few years optical detection and spectroscopy of metallic nanoparticles has also matured by a great deal, giving acees to information on single nanoparticles down to several tens of nanometers. In this talk I present a fully optical method with a sensitivity of detecting single gold clusters as small as 5nm. Furthermore, we discuss measurements on the plasmon resonances from such small particles their dependence on the shape and size of the nanoparticle. We then go on to show how single gold nanoparticles can be placed at the end of a glass fiber tip and manipulated at will in the vicinity of single fluorescent emitters. I will give a progress report on our efforts to perform controlled experiments that aim at a quantitative understanding of field enhancement phenomena.

*Half-metals for spintronics* **Room C**

### F4C1    Half-Metals: Defects and Finite Temperatures

J.J. Attema[1], L. Chioncel[2], C.M. Fang[3], G.A. de Wijs[2], A.I. Lichtenstein[2], R.A. de Groot[1]
*1) MTIN'88, Toernooiveld 1, 6525ED Nijmegen*
*2) ESM, NSRIM, Toernooiveld 1, 6525 ED Nijmegen*
*3) Solid State and Materials Chemistry, TU/e, Eindhoven, The Netherlands*

Electronic structure calculations have been playing an important role in the discovery and understanding of half-metals. Until recently calculations have been confined to zero-tempetarure. In this limit,effects of imperfections such as substitutions by foreign atoms, site interchange, vacancies, the presence of surfaces is detrimental for the spin-polarization of the conduction (or indifferent at best). Devices operate at finite temperature, however. The major challenge for computational spintronics is the inclusion of finite temperatures. We will focus on imperfections in half-metals, which are deliberately introduced in order to improve the performance at finite temperature.

### F4C2    Transition Metal Oxide based Half Metals

Zdzislawa Szotek[1]
*1) Daresbury Laboratory, Daresbury, Warrington, WA4 4AD, U.K.*

We discuss an application of the self-interaction corrected local spin density (SIC-LSD) method to half-metallic transition metal oxides, and among them double perovskites, magnetite, and such spinel ferromagnetic insulators as $NiFe_2O_4$ and $CoFe_2O_4$. We concentrate on the electronic and magnetic properties of these compounds and in magnetite, in addition, the issue of charge order is investigated. The insulating Verwey charge ordered phase is discussed in relation to the electronic structure of $NiFe_2O_4$ and $CoFe_2O_4$, of possible usage as spin filters in technological applications. We show that even such simple transition metal monoxides as MnO and NiO can acquire half-metallic characteristics when doped with cation vacancies.

*Ferromagnetic superconductors* **Room D**

### F4D1 High Pressure Studies of Superconducting Band-Ferromagnets

C. Pfleiderer[1]

*1) Physikalisches Institut, Universität Karlsruhe, D-76128 Karlsruhe, Germany*

The assumption of the existence of a quantum critical point in band-ferromagnets, notably $ZrZn_2$, has long motivated the search for ferromagnetically mediated $p$-wave pairing. However, high pressure magnetisation measurements establish, that the suppression of ferromagnetism in the superconducting band-ferromagnets $UGe_2$ and $ZrZn_2$ are discontinuous (first order), while $T_C$ even increases under pressure in URhGe. When taken together with the evidence for itinerant-electron metamagnetism the pressure dependent phase diagrams point at an important role of peaks in the density of states, suggesting that superconductivity in band-ferromagnets may be a universal phenomenon.
* work carried out in collaboration M. Uhlarz, A. D. Huxley, S. M. Hayden, F. Hardy, J. Flouquet, H. v. Löhneysen and G. G. Lonzarich

### F4D2 Electronic structure and magnetic character of $UGe_2$ and URhGe ferromagnetic superconductors

Alexander B. Shick[1]

*1) Institute of Physics ASCR, Prague*

The correlated band theory method (LSDA+U) has been applied to $UGe_2$, in which superconductivity has been found to coexist with robust ferromagnetism. Over a range of pressures, two nearly degenerate states are obtained, which differ most strikingly in uranium orbital character. The calculated moment, and its separation into spin and orbital parts, is consistent with recent polarized neutron scattering data. The calculated Fermi surface agrees reasonably with resent ARPES data. These two states are strong candidates for the two ferromagnetic phases, one low-T – low-pressure, the other higher-T – higher pressure. Magnetic waves built from fluctuations between these uranium configurations provide a possible new mechanism of pairing in $UGe_2$. A comparison between electronic and magnetic character of $UGe_2$ and URhGe will be also given.

### F4D3 Magnetism, Superconductivity and Heavy Quasiparticles in ZrZn2

S. M. Hayden[1], S.J.C. Yates[1], E. Yelland[1]

*1) H. H. Wills Physics Laboratory, University of Bristol*

$ZrZn_2$ orders ferromagnetically at $T_{FM} = 28.5$ K, with an ordered moment of $0.17\mu_B$ per formula unit at $T = 2$ K. The intrinsic moment is unsaturated, with a field of 6 Tesla causing a 50% increase. Compared with other $d$-band metals, it has an extremely large electronic heat capacity at low temperatures $C/T = 47$ mJK$^{-2}$ mol$^{-1}$. $ZrZn_2$ crystallizes in the C15 cubic Laves structure, with lattice constant $a = 7.393$ Å, the Zr atoms forming a tetrahedrally co-ordinated diamond structure. Its magnetic properties derive from the Zr $4d$ orbitals, which have a significant direct overlap.
Interest in $ZrZn_2$ has been rekindled by the discovery that it is superconducting at ambient pressure and that both the superconductivity and ferromagnetism are simultaneously destroyed by the application of hydrostatic pressure. In this talk I will present transport and magnetic data on superconducting phase and the results of recent Fermi surface studies which demonstrate to existence of strongly renormalized quasiparticles.

*Solid/liquid interfaces* **Room E**

### F4E1 Revealing the atomic structure of insulator surfaces

Michael Reichling[1]
*1) Fachbereich Physik, Universitaet Osnabrueck*

The atomic structure of insulator surfaces has for a long time not been accessible to experimental investigation as the necessary tools were not available. Recently, dynamic scannning force microscopy has been established as a method for closing this gap and atomic resolution imaging is now routine operation for several fluoride and oxide materials. For the examples of CaF2(111), CaCO3(101-4), Al2O3(0001) and CeO2(111), the state of the art in atomic resolution dynamic scanning force imaging on insulating surfaces and nanostructures is demonstrated. Individual atoms and ions and atomic scale structures can be imaged on flat terraces, step edges and metallic clusters on such surfaces. The challenges and peculiarities of atomic resolution imaging on insulators in contrast to other surfaces are outlined and it is demonstrated that we now yield a quantitative understanding of atomic contrast formation on CaF2(111).

### F4E2 Electrochemical Interfaces Studied by Nuclear Magnetic Resonance of Metals and Metallized Systems

A. Wieckowski[1]
*1) University of Illinois at Urbana-Champaign*

Tremendous research opportunities exist to study solid/liquid electrochemical interfaces when magnetic resonance of surface metal atoms and adsorbed molecules is examined. The method developed by our group to explore such opportunities, named electrochemical NMR (EC-NMR), is sensitive to chemical and electronic structure and provides spectroscopic signatures specific to surface motions. Those features, when combined with results of electrochemical measurements, enable access to information on the Fermi-level local densities of states (Ef-LDOS) of both metal surfaces and adsorbates, together with new insights into surface diffusion of electrochemical adsorbates. Detailed information then provided helps to test modern quantum theories of heterogeneous catalysis, and the measurements produce better understanding of electrochemical interfaces per se. The approach also offers new guidelines for designing better catalysts for fuel cells. Brief reports on the following issues will be made: (1) 195Pt metal NMR. (2) Ef-LDOS properties small organic molecules at metal surfaces (13C and 15N surface NMR) (3) Correlation between electronegativity of selected adsorbates and their influence on surface electronic properties platinum nanoparticles (195Pt NMR). (4) 195Pt and 13C NMR spectra of Pt/Ru nanoparticle catalysts (supported and unsupported). In this latter category, which will be highlighted as the newest one in our effort, it will be demonstrated that the Pt NMR spectrum of a Pt/Ru alloy catalyst is different from that of pure Pt. The latter extends from 1.090 G/kHz to 1.140 G/kHz reflecting homogeneous nanoparticle layered structure. In contrast, the NMR spectrum of Pt/Ru is much narrower, extending only from 1.095 G/kHz to 1.115 G/kHz, and there are few if any Pt atoms resonating in the vicinity of 1.138 G/kHz (at the 195Pt NMR frequency of bulk Pt metal). This implies that there are no Pt atoms whose electronic properties resemble those of bulk Pt. These 195Pt NMR data strongly suggest that there is a significant surface enrichment of Pt atoms in a Pt-Ru alloy nanoparticle. However, Ru is also present on the outmost layer of the Pt-Ru nanoparticles as documented before by infrared measurements [Park et al., J. Am. Chem. Soc. 125 (2003) 2282-2290]. The whole spectrum is shifted towards lower Knight shifts, indicating electronic effects due to the interaction of Pt with Ru. The analysis of the 13C spin-lattice relaxation results indicates that Ru addition causes a reduction in the Fermi level local density of states of the clean metal surface atoms and the 2pi* orbital of adsorbed CO. This shows that alloying of platinum with Ru reduces the total density of states (DOS) at the Pt sites. The ligand field contribution to the "Ru enhancement" may then be attributed to the type of the electronic alterations caused by Ru that we identified in this study. These are central issues in modern fuel cell catalysis.

F4E3    **Properties of Metal/Electrolyte Interfaces**

Klaus Wandelt[1]

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Technologically relevant processes like film growth, corrosion, catalysis etc. occur also at solid/liquid interfaces. In order to understand and optimize these processes methods are needed which provide structural and spectroscopic information from these interfaces with the same precision as in vacuum surface physics. In this contribution studies with copper single crystal electrodes will be presented using Electrochemical Scanning Tunneling Microscopy and Fourier-Transform Infrared Spectroscopy. Firstly, the atomic-scale structure of adsorbed anion layers, in particular as a function of the electrode potential, yields insight into interaction strength and charge state of the various anions. Secondly, the influence of the adsorbed anions on the gross morphology of the electrode surface will be shown and discussed. And finally the effect of the adsorbed anions on molecular processes like growth of inorganic and organic films from solution will be investigated.

### F4F1     Synthesis, electron microscopy and applications of inorganic nanotubes

Maja Remskar[1]
*1) Jozef Stefan Institute, Jamova 39, Ljubljana Slovenia*

The MoS2 and WS2 nanotubes synthesized by chemical transport reaction represent the longest known inorganic nanotubes grown up to several millimetre lengths. The nanotubes grown at nearly equilibrium conditions contain extremely low density of structural defects. They have been successfully alloyed with metals suppressing by such a manner the tube chirality and changing electrical properties. While microtubes usually grow as single tubes, the nanotubes combine some ropes formed by coaxial or side-by-side growth of primary nanotubes. The self-assembly tendency is the most obvious in the sub-nanometer MoS2-xIy nanotubes, which have been synthesised using C60 as a growth promoter. Due to the metallic behaviour these smallest known inorganic nanotubes belong to the family of promising molecular wires. The conditions of synthesis will be explained and foreseen applications will be discussed.

### F4F2     Experiments on hybrid electronics incorporating carbon nanotubes

J. Nygard[1], J.R. Hauptmann[1], A. Jensen[1], P.E. Lindelof[1], J. Sadowski[1]
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Carbon nanotubes have appeared as promising candidates for incorporation of individual molecules in nanoscale electronics. Semiconducting nanotubes can operate as high-performance field-effect transistors while metallic tubes can act as high current density wires. Moreover, low temperature electron transport has shown that new aspects of quantum transport and many body phenomena can be investigated in nanotube devices.

In most transport experiments carbon nanotubes were lying on an insulating oxide and contacted by lithographically defined electrodes made from normal metals such as gold or palladium. The task of employing carbon nanotubes in electronic applications will be easier if the nanotubes can be smoothly integrated with existing technologies such as silicon metal oxide semiconductors and III-V semiconductor heterostructures.

We present here a route where single-wall carbon nanotubes are encapsulated epitaxially in a GaAs based semiconductor heterostructure. In one type of device the nanotubes are supported by a bandgap engineered gate barrier and contacted by GaMnAs electrodes. It is shown that the nanotubes can act as interconnects between semiconductor regions and function as single-electron transistors at low temperature. However, one may envision other roles for nanotubes in electronic and optoelectronic circuits using the epitaxial encapsulation technique.

We will discuss aspects of nanotubes contacting other objects, including individual metal nanoparticles and ferromagnetic electrodes.

A. Jensen et al., Nano Letters 4, 349 (2004).

### F4F3     Ferroelectric Nanotubes and Nano-ribbons

James F. Scott[1]
*1) University of Cambridge*

A discussion will be presented on the preparation and electrical characterization of ferroelectric nanotubes and nano-ribbons (the latter are ca. 1 micron wide x 2 cm long). Both electrical transport properties and switching characteristics will be described, which differ from those in bulk or large-area planar films. Some discussion is provided of potential use in photonic arrays, in [3D] trenching of DRAMs and related memory devices, and in the piezoelectrically driven micro-fluidics applications. The relationship with the International "Road Map" for non-volatile FRAM memory development is detailed.

*Giant piezoelectricitys* **Room G**

### F4G1 Origin of Giant Electrostriction and Piezoelectricity in Relaxors

R. Blinc[1], R. Pirc[1], B. Zalar[1], V. Laguta[1]
*1) J. Stefan Institute, 1000 Ljubljana, Slovenia*

Relaxor ferroelectrics are characterized by a large electrostrictive response and giant piezoelectricity in an applied electric field. So far the microscopic origin of these phenomena has not been fully understood. Here we investigate the role of polar nanoregions - which are known to exist in relaxors - in electrostrictive and piezoelectric phenomena. First we present some recent evidence for the existence of disorder in classical perovskites like $BaTiO_3$, $SrTiO_3$ and $KTaO_3$: Nb and polar nanoclusters in PMN relaxors. Within the framework of the spherical random bond random field model, where the interaction between polar nanoregions is modulated by a lattice stress, an expression for the electrostrictive and piezoelectric coefficients is obtained and the results are compared with the experimental data. The polarization rotation mechanism believed to be responsible for the ultrahigh piezoelectric response in mixed PZN PT and PMN PT single crystals is as well discussed. Recent measurements of the nanocluster dynamics are presented.

### F4G2 Giant electro-strain by point-defect-mediated reversible domain switching

Xiaobing Ren[1]
*1) National Institute for Materials Science Tsukuba, Ibaraki 305-0047, Japan*

Piezoelectricity (electric-field induced strain) has found extensive applications in actuators and sensors. However, the effect is generally very small and thus limits its usefulness. Here I show that with a different mechanism, an aged $BaTiO_3$ single crystal can generate a large recoverable non-linear strain of 0.75% at a low field of 200V/mm, which is about 40 times higher than piezoelectric PZT ceramics and more than 10 times higher than the high strain PZN-PT single crystals. This giant electro-strain stems from an unusual point-defect-mediated reversible domain switching mechanism. This mechanism provides a general method to achieve large electro-strain effect in a wide range of ferroelectric systems and the effect may lead to novel applications in ultra large-stroke and non-linear actuators.

### F4G3 Theory of polarization rotation in relaxor ferroelectrics

RE Cohen[1]
*1) Carnegie Institution of Washington*

New single crystal piezoelectrics such as PMN-PT and PZN-PT show strains of up to 2% in an applied field, and have shown about 10 times the electromechanical coupling as current generation ceramics. Their large coupling can be understood as due to polarization rotation in an applied field (Fu and Cohen, Nature 403, 281 2000). In convention ferroelectrics like $PbTiO_3$ (PT), the polarization direction is fixed, giving rise to relatively small electromechanical coupling. However, PT has a huge tetragonal strain of 6%. Rhombohedral ferroelectrics like rhombohedral BT have very small strains. If there was a rhombohedral phase for PT, one could obtain a huge electromechanical response by driving a phase transition from rhombohedral, with the polarization along [111], to tetragonal, with the polarization along [001], i.e. by rotating the polarization. This is the mechanism of relaxor ferroelectrics like PMN-PT. We are using a multiscale first-principles approach to study relaxor-ferroelectrics.

*Microcavities* **Room H**

F4H1 **Microcavity polariton dynamics in the linear and non-linear regime**

Wolfgang Langbein[1]
*1) Experimentelle Physik IIb, Universitaet Dortmund, Otto-Hahn Str. 4, 44227 Dortmund, Germany*

In planar semiconductor microcavities, the photonic part of cavity polaritons makes them easy to access by optical means, while their excitonic part enables strong mutual non-linear interaction. The polariton dynamics in a III-V microcavity is investigated using time-resolved imaging of the emission in real or reciprocal space. Using real-space imaging, propagation of polaritons after point-like injection is found. Free propagation over hundreds of micrometers is observed. Structured regions allow polariton guiding and coherent scattering. Using directional imaging, a dynamical narrowing of the disorder-scattered ring-shaped polariton distribution in momentum space is demonstrated, in agreement with the time-energy uncertainty limit, and a finite directional width of the polariton states is observed. At higher excitation intensities, parametric polariton-polariton scattering is observed. Moreover, the quantum-mechanical complementarity principle is demonstrated for parametrically scattered polariton pairs.

F4H2 **Polariton stimulation and condensation in semiconductor microcavities**

Maxime Richard[1], Jacek Kasprzak[1], Regis Andre[1], Robert Romestain[1], Le Si Dang[1]
*1) Universite Joseph Fourier - Grenoble*

Exciton-polaritons are bosonic eigenstates of semiconductor microcavities, consisting of a coherent mixing of quantum well excitons and cavity photons. They are better candidates for bosonic condensation than excitons since their density of states is four orders of magnitude smaller. Previous experimental studies of CdTe microcavities have clearly demonstrated that stimulated emission of polaritons can be obtained under non-resonant optical excitation. In this work, we present an experimental study of CdTe polaritons in this high excitation regime. An angle-resolved spectroscopy setup has been used to probe the polariton population along the dispersion curve. In the high excitation regime, the population distribution is found to be strongly peaked at small k// states by stimulated relaxation process, with a completely flat dispersion. We show that the anomalous dispersion could be explained in terms of coherent collisions between in-phase polaritons.

*Structural studies of lowdimensional nanostructures* **Hall J**

F4J1 **Magnetization reversal in magnetic nanostructures studied by neutron reflectivity**

K. Temst[1], M.J. Van Bael[1], J. Swerts[1], H. Loosvelt[1], E. Popova[1], C. Van Haesendonck[1], H. Fritzsche[2], M. Gierlings[2]

*1) Laboratorium voor Vaste-Stoffysica en Magnetisme, K.U. Leuven, Celestijnenlaan 200 D, B-3001 Leuven, Belgium*
*2) Hahn-Meitner-Institut, Glienicker Strasse 100, D-14109 Berlin, Germany*

In this contribution we review recent work on the study of magnetic domain states and magnetization reversal in patterned magnetic nanostructures using polarized neutron reflectivity techniques. Polarized neutron reflectivity has the unique advantage that it can provide direct information about the magnetization reversal mechanism since it probes simultaneously magnetization components parallel and perpendicular to the applied field. We will report here on the study of magnetization reversal and the influence of shape anisotropy in ferromagnetic dots and lines, as well as patterned exchange-bias structures.

F4J2 **Limits and prospects of x-ray scattering from self-organized epitaxial nanostructures**

V. Holý[1], [1]

*1) Department of Electronic Structures, Charles University, Ke Karlovu 5, 121 16 Prague, Czech Republic*

X-ray scattering methods are frequently used for a non-destructive structural characterization of semiconductor nanostructures (quantum wires and dots) prepared by a self-organization growth method. The application of these methods is complicated due to very small volumes of the nanostructures. In order to enhance the useful signal and to suppress the substrate background, small-angle scattering and diffraction in a grazing-incidence scattering geometry are used; then, the penetration depth of the incoming x-ray beam is limited down to few nm. The methods are indirect, i.e., the experimental results have to be compared with numerical simulations based on a suitable structure model. Direct methods determining the shape and chemical composition of the nanostructures use, among others, anomalous scattering effects occurring close to an absorption edge. In the talk, experimental results are reviewed obtained from various types of the nanostructures and a possible further development of x-ray scattering methods in this field is discussed.

# Plenary Session 10:30 – 12:00 Hall A

P4A1  **<u>Magnetic Semiconductors</u>**

Tomasz Dietl[1]

*1) Institute of Physics, Polish Academy of Sciences and ERATO Semiconductor Spintronics JST Project, al. Lotnikow 32/46, PL-02668 Warszawa, Poland*

Recent years have witnessed enormous progress in understanding the nature of the carrier-controlled ferromagnetism in diluted magnetic semiconductors to the point that (Ga,Mn)As, p-(Cd,Mn)Te, and related compounds appear as the best understood ferromagnets. At the same time, isothermal and reversible magnetization switching by light, electric field and current has been demonstrated at low temperatures showing potential functionalities of these systems. Particularly promising are magnetically doped group III nitrides and group II oxides, in which spontaneous magnetization is found to persist above the room temperature. However, we are still at the beginning of the road to understanding and controlling doping, defects, and magnetism in these wide gap magnetic semiconductors.

# Mini-Colloquia 14:00 – 16:00

*Novel phenomena in atomic quantum gases* **Room B**

M4B1 **Bose-Einstein condensation of $^6$Li$_2$ molecules and the BEC-BCS crossover**

S. Jochim[1], M. Bartenstein[1], A. Altmeyer[1], S. Riedl[1], G. Hendl[1], C. Chin[1], J. Hecker Denschlag[1], R. Grimm[2]

*1) Institut für Experimentalphysik, Universität Innsbruck, Technikerstrasse 25, 6020 Innsbruck, Austria*

*2) Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, 6020 Innsbruck, Austria*

We report on the Bose-Einstein condensation of more than $10^5$ Li$_2$ molecules in an optical trap starting from a spin mixture of fermionic lithium atoms [1]. During forced evaporative cooling, the molecules are formed by three-body recombination near a Feshbach resonance and finally condense in a long-lived thermal equilibrium state. The pure molecular condensate is then used to investigate the BEC-BCS crossover with various methods.

[1] S. Jochim et al., Science 302, 2103 (2003); Published online 13 November 2003; 10.1126/science.1093280

M4B2 **Resonance effects on the crossover of bosonic to fermionic superfluidity**

Maria Luisa Chiofalo[1], Stefania De Palo[2], Murray J. Holland[3], Servaas Kokkelmans[4]

*1) INFM and Classe di Scienze, Scuola Normale Superiore, Pisa, Italy*

*2) Dip. di Fisica and INFM, Universita' di Roma "La Sapienza", Italy*

*3) CRS-BEC INFM and Dipartimento di Fisica, Universita' di Trento, Povo, Italy*

*4) Eindhoven University of Technology, Eindhoven, The Netherlands*

Feshbach scattering resonances are being utilized in atomic gases to explore the entire crossover region from a Bose-Einstein Condensation (BEC) of composite bosons to a Bardeen-Cooper-Schrieffer (BCS) of Cooper pairs.

After overviewing the main issues concerning the theoretical description of the crossover physics, the attention is focused on the conditions for universal behaviour of the thermodynamic quantities near resonance. We point out that in the general case of narrow Feshbach resonances the universal picture fails and show how the energy dependence of the scattering phase shift does affect the emergence of the superfluid state.

M4B3 **Overview**

Anthony J. Leggett[1]

*1) Dept.of Physics,University of Illinois,1110 W.Green St.,Urbana,IL 61801*

I attempt to review some of the most exciting recent developments in the field of dilute atomic alkali gases,with particular emphasis on experiments in optical lattices and on the "BEC-BCS crossover problem". I will try to pinpoint some of the most urgent outstanding conceptual issues.

*Physics of f-electron materials IV. (PCFES 7)* **Room C**

M4C1 **Avoided Antiferromagnetic Order and Quantum Critical Point in CeCoIn$_5$**

A. D. Bianchi[1], R. Movshovich[1], I. Vekhter[1], P. G. Pagliuso[1], J. L. Sarrao[1]
*1) Los Alamos National Laboratory, Los Alamos, NM 87545, USA*

We measured the specific heat $C_p(T)$ and resistivity $\rho(T)$ of heavy fermion CeCoIn$_5$ between the superconducting critical field $H_{c2}$ = 5 T and 9 T, with the field $H$ in the [001] direction, and temperatures down to 50 mK. These results show that this compound has a quantum critical point (QCP) with the magnetic field as tuning parameter. For a field of 5 T, just above $H_{c2}$, the $T$-dependence of both $C_p(T)$, and $\rho(T)$ show non-Fermi liquid (NFL) behavior down to the lowest $T$ with $C_p(T) \propto -\log(T)$ and $\rho(T) - \rho(T = 0) \propto T$. For $H$ above 8 T the data exhibit a crossover from FL to a NFL behavior. $C_p(T)$ and $\rho(T)$ data show scaling behavior predicted by spin-fluctuation theory, suggesting that the NFL behavior is due to incipient antiferromagnetism (AFM) in CeCoIn5 with the QCP in the vicinity of $H_{c2}$. For fields below $H_{c2}$ the AFM phase separated by a QCP from the paramagnetic ground state is not observed, as the system becomes first superconducting.

M4C2 **Microscopic approach to superconductivity and magnetism of 115 compounds based on a j-j coupling scheme**

Takashi Hotta[1]
*1) Advanced Science Research Center, Japan Atomic Energy Research Institute*

In order to understand the mechanism of superconductivity and magnetism of f-electron materials with HoCoGa$_5$-type tetragonal crystal structure, first we have performed fully relativistic band-structure calculations to clarify electronic structure and Fermi surface of 115 systems. Then, we have constructed a microscopic model based on a j-j coupling scheme. Analyzing the model with the use of various kinds of theoretical techniques, we have attempted to clarify the mechanism of superconductivity and magnetism of 115 compounds. In this talk, the band-structure calculation results for AnTGa$_5$ (An=U, Np, Pu; T=Fe, Co, Ni) will be introduced. Then, we will show our recent results on superconductivity and magnetism of 115 compounds by focusing on hidden orbital ordering and potential role of orbital fluctuations.

M4C3 **Magnetic structure of UTGa$_5$ and NpTGa$_5$**

N. Metoki[1]
*1) Advanced Science Research Center, JAERI*

The family of '115' system presents the variety of electronic and magnetic properties including heavy fermion superconductors CeTIn$_5$ and PuTGa$_5$. High quality single crystals can be grown systematically with different number and character of $f$ electrons and transition metal $d$-electrons. Many UTGa$_5$ exhibits Pauli-paramagnetic behavior due to the strong itinerant character of $5f$ electrons hybridized with Ga $4p$ band. Meanwhile NpTGa$_5$ favors magnetically ordered ground state. In this talk, the magnetic structure of UTGa$_5$ and NpTGa$_5$ will be reported. We show that the magnetic stucture of the iso-electronic UTGa$_5$ for T=Ni, Pd, Pt is controlled by the local symmetry at uranium site, where the orbital degree-of-freedom would play important role for the magnetic interaction. NpTGa$_5$ with different $d$-electron number (T=Fe, Co, Ni) showed variety of magnetic structure with G-, C-, A-type antiferromagnetic and ferromagnetic order. The transition metal element possesses magnetic moment in NpFeGa$_5$ and possibly NpNiGa$_5$.

M4C4    **Heat and Charge Transport at at Field-Tuned Quantum Critical Point**

Johnpierre Paglione[1], M. A. Tanatar[1], D. G. Hawthorn[1], E. Boaknin[1], R. W. Hill[1], F. Ronning[1], M. Sutherland[1], S. Li[2], Louis Taillefer[2], C. Petrovic[3], P.C. Canfield[4]

*1) Department of Physics, University of Toronto, Toronto, Canada*
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In the vicinity of a quantum phase transition, corrections to the standard theory of metals (Fermi-liquid theory) are needed to account for the anomalous properties of electrons, such as an electrical resistivity that grows linearly with temperature or an effective mass that diverges with decreasing temperature. Nevertheless, the basic excitations of the electron system in the limit of zero energy (or temperature) are still thought to be Landau quasiparticles  spin-1/2 fermions carrying one unit of charge. A robust property of such excitations is expressed as the Wiedemann-Franz (WF) law: heat and charge are transported with perfectly equal ability. But what happens when zero-point, or quantum critical, fluctuations dominate the energy spectrum? In the heavy-fermion material $CeCoIn_5$, the observed divergence of the $T^2$ coefficient of the resistivity with magnetic field has recently revealed a new quantum critical point (QCP) [1]. Here we compare heat and charge transport in $CeCoIn_5$ in the vicinity of the QCP. This allows us to 1) test the WF law at $T \to 0$, and 2) shed light on the momentum dependence of the critical inelastic scattering at finite temperature.

[1] J. Paglione et al., Phys. Rev. Lett. 91, 246405 (2003).

*Role of spin in quantum transport*       **Room D**

M4D1    **Conditions for Adiabatic Spin Transport in Disordered Systems**

Diego Frustaglia[1], Markus Popp[2], Klaus Richter[3]
*1) Scuola Normale Superiore, Pisa, Italy*
*2) Max-Planck-Institut für Quantenoptik, Garching, Germany*
*3) Institut für Theoretische Physik, Universität Regensburg, Germany*

We address the controversy concerning the necessary conditions for the observation of Berry phases in disordered mesoscopic conductors [1-5]. For this purpose, we calculate the spin-dependent conductance of disordered two-dimensional structures in the presence of inhomogeneous magnetic fields. Our numerical results [6] show that for both, the overall conductance and quantum corrections, the relevant parameter defining adiabatic spin transport scales with the square root of the number of scattering events, in generalization of Stern's original proposal [1]. This could hinder a clear-cut experimental observation of Berry phase effects in diffusive rings.

[1] A. Stern, PRL **68**, 1022 (1992).
[2] D. Loss, H. Schoeller, and P.M. Goldbart, PRB **48**, 15218 (1993).
[3] S. van Langen, H. Knops, J. Paasschens, and C. Beenakker, PRB **59**, 2102 (1999).
[4] D. Loss, H. Schoeller, and P.M. Goldbart, PRB **59**, 13328 (1999).
[5] H.-A. Engel and D. Loss, PRB **62**, 10238 (2000).
[6] M. Popp, D. Frustaglia, and K. Richter, PRB **68**, 041303(R) (2003).

M4D2    **Role of nuclear spins in quantum dots**

Yu.V. Nazarov[1]
*1) Kavli Institute of NanoScience Delft, Delft University of Technology*

We review the research of Delft theory group that concerns interaction of electron and nuclear spin in quantum dots. We concentrate on semisclassical effective-field approach and discuss why it is valid. We describe how nuclear spins facilitate singlet-triplet transitions and transitions within spin doublet, and reveal unusual dynamics of nuclear magnetization in the field of electron spin. We present a model to understand very slow current oscillationds in the spin-blockade regime, those have been observed experimentally (cond-mat/0309062).

M4D3    **Magnetic Bipolar Transistor**

Jaroslav Fabian[1], Igor Zutic[2]
*1) Institute for Physics, Karl-Franzens University Graz*
*2) Condensed Matter Theory Center and University of Maryland at College Park, Center for Computational Materials Science, NRL Washington DC*

A novel semiconductor device concept–magnetic bipolar transistor [1]–in which one of the active semiconductor regions is magnetic, is shown to exhibit several useful phenomena. These include extrinsic and intrinsic spin injection, as well as normal and giant magnetoamplification effects. Analytical modeling of the magnetic transistor will be discussed and a qualitative reasoning will be given to understand the new effects. The transistor has potential as a spintronic device [2] for magentic sensing and nonvolatile information storage.

[1] J. Fabian and I. Zutic, Phys. Rev. B 69, 115314 (2004)
[2] I. Zutic, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004)

*Entropic forces* **Room E**

M4E1 **Depletion forces in purely entropic systems**

Laurent Helden[1], Clemens Bechinger[1]
*1) 2. Physikalisches Institut, University of Stuttgart, Germany*

The stability and phase behavior of colloidal suspensions containing particles of different size and shape is known to be strongly influenced by depletion forces. Such depletion forces can lead even in systems where the pair interaction is purely repulsive to attractive forces which may finally cause particle flocculation. Accordingly, the understanding of these forces is besides fundamental interest also essential for industrial processes.

Here we present direct measurements of the depletion interaction potentials between a spherical colloidal probe particle and a flat surface in the presence of various depletion agents. Results were obtained by the technique of total internal reflection microscopy (TIRM) which allows high precision measurements with a force resolution below 10 fN.

M4E2 **Polymer-colloid mixtures: the dark hand of entropy**

Ard Louis[1]
*1) Department of Chemistry, Cambridge University*

Polymer colloid mixtures pose a classic multiple length scale problem: Whereas the colloids can easily be viewed as single "giant atoms", the polymers are typically modelled by hundreds or even thousands of small constituents, all strung together. When the polymer radius of gyration $R_g$ is much smaller than the colloidal radius $R_c$, the behaviour of the mixture can be accurately described using effective depletion pair potentials. But in the opposite "protein limit", where $R_g/R_c >> 1$, the pair potential approximation breaks down qualitatively. In this talk we will discuss
**a)** a quantitative semi-analytical form for the depletion potential for polymers in good and theta solvents.
**b)** a coarse-graining technique, "polymers as soft colloids", to treat polymer colloid mixtures.
**c)** polymer-colloid mixtures in the "protein limit", where $R_g/R_c >> 1$.

M4E3 **The interface in a phase separated colloid-polymer mixture**

D. G. A. L. Aarts[1], H. N. W. Lekkerkerker[1]
*1) Van 't Hoff Laboratory, Debye Research Institute, University of Utrecht*

Mixtures of colloids and polymers display a rich phase behavior, involving colloidal gas (rich in polymer, poor in colloid), colloidal liquid (poor in polymer, rich in colloid) and colloidal crystal phases (poor in polymer, highly ordered colloids). Here we studied by means of confocal scanning laser microscopy a gas-liquid phase separating mixture of small fluorescent polymethylmethacrylate (PMMA) spheres and polystyrene polymer in decalin. We show results for the free interface and for the mixture near a single hard wall. Due to the colloidal length scale the interfacial tension is much lower than in the molecular analog ($\mu$N/m in stead of mN/m). This low interfacial tension has pronounced effects on the interface fluctuations and the colloidal gas-liquid profile near a single wall. We show that the fluctuations can be described within the capillary wave model and that the interplay between hydrostatic and Laplace pressure accurately describes the profile at a single hard wall. The liquid phase has a clear tendency to wet the wall completely.

*Interaction of matter with laser light under extreme conditions* **Room F**

M4F1 **Particle acceleration from laser-created relativistic plasmas**

P.V. Nickles[1], M. Schnurer[1], S. Ter-Avetisyan[1], S. Bush[1], A. Kemp[2], D. Hilscher[3], U. Janke[3], W. Sander[1]
*1) Max-Born-Institute, Berlin*
*2) University Reno, Nevada*
*3) Hahn-Meitner Institute, Berlin*

The recent ultra-short and highly intense laser development using the CPA- (chirped pulse amplification) techniques has opened new perspectives of laser driven particle acceleration relying on the fact that a small volume of matter can be highly excited with ultrashort intense light pulses using only a moderate amount of energy. The laser pulse energy is efficiently transferred to hot electrons. They build up a strong charge field which in turn can accelerate ions to high energies. These fast moving ions with kinetic energy of several tens of MeV carry a significant part of the incident laser energy. This has actuated a broad variety of work concerning the underlying physics and possible applications. Especially proton beams with energies of several MeV are in the focus since they have potential for the proton imaging of dense plasmas or structured matter. We report on experimental studies, where small (20 $\mu$m) water and heavy water droplets have been exposed with relativistically intense ($\sim 10^{19}$ W/cm$^2$) laser pulses in order to study ultrashort ($\sim 40$ fs) laser pulse driven ion acceleration. These droplets can be produced with a high repetition rate, are cheap and have the advantage to be an isolated structure. The outward directed acceleration of the ions (deuterons) in the dense spherical plasma was studied using an array of up to four Thomson spectromaters and recording the ion spectra in a single shot. The "in-flight" ion acceleration could be measured in an indirect way employing the fusion neutrons produced by deuterons with energies above 10keV according to the famous D(d,n) reaction. Four neutron-TOF spectrometers were used to measure the absolute neutron yield and angular distribution. The diagnostics developed allowed to record correlated data about the ion emission and the neutron spectra.The results bring a new insight into the ion acceleration with relativistically intense and extremely short laser pulses and might be useful for the problem of tailoring the ion beam spectra to reach "monoenergetic" ion beams from laser produced plasma in the future.

M4F2 **Equation of State measurements and Phase Transitions in the Megabar regime with laser-driven shock waves**

Dimitri Batani[1], Michel Koenig[2], Alessandra Benuzzi-Mounaix[2], Tom Hall[3]
*1) Dipartimento di Fisica "G.Occhialini", Universit? di Milano-Bicocca, Italy*
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In recent years laser-driven shocks have become a reliable tool for Equation of State measurements in the Megabar and Multimegabar regime. This has been possible thanks to improvements in the uniformity of energy deposition and in control of target preheating, as well to developments in experimental diagnostics. Phase transitions were evidenced by using new diagnostics with high spatial and temporal resolution. In particular measurements of material reflectivity allow electrical conductivity to be evaluated, evidencing the occurrence of metallic transitions. These measurements are useful both in the context of Inertial Confinement Fusion where pellet materials are compressed to very high densities, and for astrophysics and planetology. Indeed laser driven shocks allow reproducing in laboratory the conditions found in the interior of giant planets and dwarf stars.
In this context, we present some recent experimental results on iron, which is important for understanding the interior of the Earth, and of water and carbon, which are relevant to the study of the structure of planets like Uranus and Neptune, and for explaining the origin of their large magnetic field. Experimental results have been obtained in various laser facilities including LULI (France), Rutherford Lab. (England), PALS (Prague, Czech Rep.).

M4F3 **Interferometry applications of X-ray lasers at LIXAM. Diagnostics of surfaces and plasmas using X-ray lasers. Recent progress and perspectives : towards to the future LASERIX facility of LIXAM**

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In this paper we will review our experimental activity about the utilization of X-ray lasers for interferometry applications. This work concerns both QSS and transient X-ray lasers; it involves a number of French and international collaborations and was carried out with different pump laser facilities: at JAERI (in Japan), at PALS (in the Czech Republic) and at LULI (in France). We will first present the result of diagnostic surfaces under high electric field performed at LULI and PALS. We will then describe experiments of laser-induced plasma, based on bi-mirror interference microscopy (developped at LCFIO) and performed at JAERI with a transient soft X-ray laser at 14 nm. Finally we will describe the status of the French project LASERIX, which will be especially devoted to the development of XUV lasers and their applications, and will be open to the scientific community.

M4F5 **The production of extreme ultra-violet laser radiation by optical laser irradiation of solid targets**

Greg Tallents[1]
*1) University of York*

High power laser irradiation of solid targets in a line focus can generate extreme ultra-violet laser action along the line. Typically a pre-pulse generates an expanding plasma into which a pumping laser pulse is incident. The plasma is ionised to the Ne-like or Ni-like ionisation stage depending on the atomic number of the solid target and lasing occurs between excited sub-shells by amplified spontaneous emission without mirrors. Record short wavelengths down to 5.8 nm have been observed to exhibit saturated lasing where stimulated emission becomes a significant depletion process on the upper lasing quantum state. In this talk, recent experimental work on the development of extreme ultra-violet lasers undertaken using the VULCAN laser at the Rutherford Appleton Laboratory is reviewed and compared to detailed simulations. Applications and limitations of extreme ultra-violet lasers are considered.

*Structure and dynamics of disordered ferroelectrics* **Room G**

## M4G1 The microscopic origin of relaxor ferroelectricity

Annette Bussmann-Holder[1]
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The phenomenon of relaxor ferroelectricity remains under intense research, since neither its microscopic origin could be identified unambiguously, nor could the related technologically interesting properties be related to the composition of the underlying materials. Here it is shown, that the relaxor behaviour can be understood, by modelling it as composite of soft matter diluted by highly polarizable impurities. The diluting impurities act as dipole centers which create strain fields in the host matrix accompanied by compensating dipoles. The length scales of these compensating fields depends on the temperature/strength of the induced dipole and typically defines mesoscopic regions. The substantial nonlinearity, related to this problem, induces breather type excitations which couple to the host lattice displacement fields and prohibit mode softening together with guaranteeing lattice stability. The modelling of relaxors in terms of a superposition of nonlinear excitations and conventional lattice dynamics provides a natural explanation for the broad frequency dependent dielectric response, the diffuseness of any phase transition and the proximity of relaxors to ferroelastically soft matter. In addition the relationship to glassy systems, often argued to be the origin of relaxors, can be derived on microscopic grounds.

## M4G2 Morphotropic phases in PSN-PT : bulk and thin film

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Relaxor-based compounds have attracted many attentions because of their high dielectric permittivity or their giant electromechanical coefficients. In relaxor-PbTiO3 systems such as PMN-PT, PZN-PT these outstanding properties have been connected to the so-called morphotropic phase boundary corresponding to a monoclinic structure. We have recently shown (ref) the existence of a monoclinic phase in bulk PSN-PT. In this conference we will present a comparative study between ceramic and thin films deposited on SrTiO3 and MgO.
Ref :R. Haumont, B. Dkhil, J.M. Kiat, A. Al-Barakaty, H. Dammak, L. Bellaiche, Phys. Rev. B, 68, 014114, 2003

## M4G3 Investigation of polar structure in PMN-PT relaxors via Piezoresponse Force Microscopy

Vladimir Shvartsman[1], Andrei Kholkin[1]
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Relaxors attract significant interest due to their excellent dielectric and piezoelectric properties. The peculiar properties of relaxors are attributed to the formation of nano-sized polar regions. Recently, the Piezoresponse Force Microscopy (PFM) has been successfully applied for the investigation of ferroelectric materials at the nanoscale. We report the results of high-resolution domain studies in 0.8Pb(Mg1/3Nb2/3)O3-0.2PbTiO3 single crystals via PFM. The complex structure consisting from microsized domain containing inside the small nanodomains of opposite orientation was revealed. The existence of such structure is related to the combination of relaxor and ferroelectric properties in this composition. The microdomains are usual ferroelectric domains, while the nanodomains are considered as polar nanoregions existed above the phase transition temperature and been preserved due to variation of local random fields.

M4G4 **Soft mode behaviors in induced ferroelectric states in quantum paraelectric SrTiO3 and KTaO3**

Yoshiaki Uesu[1], Yasusada Yamada[1]
*1) Department of Physics, Waseda University*

Temperature dependences of the lowest-lying TO phonon of O18 replaced SrTiO3 with its critical concentration of 0.33 and KTaO3 at Li-impurity concentration of 0.03 were investigated by neutron inelastic scattering. Against anticipation, we found that no substantial changes were observed in both crystals in comparison with pure substances. This indicates that that the critical softening of the mode is not the driving mechanism of the induced ferroelectric state, and the origin is attributed to the order-disorder mechanism of related atoms. Detail experimental results will be presented together with the interpretation.

M4G5 **Lattice Dynamics of Relaxor Ferroelectrics**

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*2) University of Tennessee*

Relaxor ferroelectric oxides show a diffuse and frequency dependent maximum of dielectric susceptibility at Tg, but local ferroelectric polarization persists well above Tg up to the Burns temperature, Td. The nature of the transition at Td and the mechanism of relaxor phenomena are still controversial. We carried out inelastic neutron scattering studies with the time-of-flight spectrometer Pharos to examine the lattice dynamics of Pb(Mg1/3Nb2/3)O3 (PMN) as a function of temperature. The data were analyzed to obtain the dynamic structure factor and dynamic pair-density function (PDF). It was found that at temperatures above Td the dynamics of oxygen and lead are decoupled, and lead sees an average, undistorted environment. Below Td they become dynamically coupled, gradually slow down and freeze at Tg. This result explains the relaxor behavior in terms of interplay between random ionic position and atomic dynamics.

M4G6 **Disorder and Phase Transitions in Classical Perovskites and Relaxors**

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*3) Tokyo Institute of Technology, Yokohama, Japan*

Classical displacive ferroelectrics like BaTiO3,SrTiO3 (STO)and isotopically enriched STO-18 have been recently shown to contain a significant order-disorder componenti in the cubic phase. Ti ion disorder is present also in the tetragonal phases. Here we report on the interplay between the soft mode and the disorder components in the phase transtion mechanisms in these systems as well as on the structural changes occuring at the ferroelectric phase transition at Tc = 24 K in SrTiO3-18. In particular we show that the appearance of a non-zero value of the asymmetry parameter of the electric field gradient tensor at the Sr site in STO-18 demonstrates the lowering of the tetragonal symmetry below Tc. The implications of this disorder for relaxors like PMN are discussed.

M4G7    **Structure and dynamics of uniaxial relaxor ferroelectrics**

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*2) Physics Department, University of Vilnius, Vilnius, Lithuania*

Owing to intrinsic charge disorder the uniaxial ferroelectric crystal strontium-barium-niobate (SBN) materializes the 3D ferroic random-field Ising model (RFIM) as evidenced, e.g., by its critical behavior and by the occurrence of a zero-field cooled ferroelectric nanodomain state. Above $T_c \sim$ 350 K the dynamics of nanopolar regions is characterized by broad steps and peaks, respectively, of the dielectric susceptibility components at $10^6 <$ f $< 10^9$ Hz. In agreement with the 3D RFIM the largest relaxation time obeys activated dynamic scaling, viz. a Vogel-Fulcher law with a dynamic exponent $> 1$. Close to $T_c$ an ultraslow central peaklike anomaly due to critical cluster relaxation lies between the regimes of domain wall creep (f $< 1$ Hz) and segmental relaxation (f $> 1$ Hz). The latter processes dominate the aging of the domain state below $T_c$, whose ergodicity breaking differs when substituting A and B sites by $Ce^{3+}$ and $Cr^{3+}$, respectively.

M4G8    **Phonons and central mode behaviour in $PbMg_{1/3}Nb_{2/3}O_3$ and $PbSc_{1/2}Ta_{1/2}O_3$ relaxor ferroelectrics**

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*2) Ceramics Laboratory, EPFL, 1015 Lausanne, Switzerland*

Peculiar dielectric properties of relaxor ferroelectrics are connected with a broad dielectric relaxation (central mode) below the phonon frequencies stemming from the dynamics of polar nanoclusters. The main dielectric dispersion near room temperature is concentrated into the microwave range. Relaxation frequency softens on cooling and simultaneously the distribution of relaxation frequencies broadens. FIR transmission measurements of PMN and PST thin films (both ordered and disordered), performed up to 900 K, show optic soft mode behaviour and central mode which comes to THz range above room temperature, merges with the soft mode and disappears from the spectra above the Burns temperature (600 K). Origin of the phonon waterfall will be discussed.

M4G9    **Liquid crystalline phases formed by nonchiral bent-shaped molecules**

Milada Glogarová[1]
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Liquid crystals composed of bent-shaped molecules are the subject of extensive investigation during the last years. In contrast to conventional liquid crystals built of rod-like molecules, in these systems the polar order can exist even for the non-chiral molecules, the antiferroelectric order being strongly preferred. The molecular dipoles directed along the transverse molecular axes are ordered because of the close packing of bent-shaped molecules within the smectic layers, hindering their rotation along the long axes. These materials exhibit new types of mesophases with no analogues among the classical calamitic phases. Phases with overall racemic and chiral symmetries are formed, both having the dipolar order. The phase with liquid-like smectic layers (denoted B2), which exhibits four variants with different symmetry, is the most promising for optical and electrooptical applications. Its textures and structures and behavior in the electric field are discussed.

M4H1 **Electron - phonon scattering and acoustic vibrations in metal clusters**

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With the advance of femtosecond lasers, time-resolved optical techniques have emerged as powerful tools for the investigation of the electronic and vibrational kinetics of matter. In metals, femtosecond techniques provide the opportunity to separate in the time domain the different electron scattering mechanisms, and to monitor acoustic processes. In time-resolved pump-probe experiments, energy is first selectively injected in the conduction electrons by a femtosecond pulse. Their relaxation kinetics is subsequently followed by monitoring the time-dependent optical response of the sample with a probe pulse. We will discuss the electron-lattice energy exchanges in small noble metal nanoparticles (gold and silver clusters, with sizes ranging between 30nm and 2nm). Experimental results show a strong increase of the electron-phonon interactions for sizes smaller than 10nm, due to a confinement effect. These fast energy exchanges leads to an ultrafast heating of the lattice, launching low frequency quantified vibrational modes. We will show that the fundamental and high order radial modes can be launched and detected, permitting precise measurements of their characteristics (period and damping).

M4H2 **Electron-hole relaxation dynamics and time-resolved optical-phonon emission in ZnCdTe quantum wells and quantum dots**

Pierre Gilliot[1], Steeve Cronenberger[1], Yannick Viale[1], Mathieu Gallart[1], Bernd Hoenerlage[1]
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We present a study of Cd-rich ZnCdTe islands confined along the growth direction by pure ZnTe barriers and laterally by Zn-rich ZnCdTe QWs. Using time-resolved pump-and-probe and four-wave mixing spectroscopy, we determine the population and dephasing dynamics of excitons at low temperature. After excitation of the Zn-rich CdZnTe quantum wells, the emission of a phonon cascade, with an energy corresponding to that of the QWs, occurs. When exciting selectively with spectrally narrow pulses, we are able to measure the dynamics of this exciton relaxation and we determine the time which is necessary for the emission of the optical phonon to be 100 fs. Following the trapping of the electron-hole pairs in the Cd-rich islands, we observe the relaxation between coupled exciton-phonon QD states by emission of phonons of the QDs, with a time constant of 25 ps. We show that this process strongly determines the dephasing dynamics of the excitons. The dephasing time of the transition from the unexcited QDs ground state is thus strongly shortened, if compared to the transition from the lowest excited QDs state which is observed in photoluminescence experiments.

M4H3 **Ultrafast Spin Dynamics in Antiferromagnetic Materials**

Andrei Kirilyuk[1]
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Antiferromagnetic (AFM) materials, though representing the overwhelming majority of magnetically ordered materials, for a long time remained an issue of academic interest only, in contrast to ferromagnets. The fundamental difference between the two types of magnetic materials manifests itself in their reaction to an external magnetic field that originates from the fact that in an antiferromagnet, the exchange interaction leads to zero net magnetization. The related absence of a net angular momentum results in an orders of magnitude faster AFM spin dynamics. In this I will discuss how the spins of an antiferromagnet can indeed be manipulated with a laser pulse via a change in lattice temperature on a time scale of a few picoseconds, in contrast to the hundreds of ps in a ferromagnet. The ultrafast dynamics of spins in antiferromagnets may be thus able to revolutionize the now limited set of applications for the AFM materials.

M4H4    **Tailoring ultrafast carrier dynamics in CdSe and CdS nanocrystalline films prepared by chemical bath deposition**

P. Nemec[1], M. Simurda[1], F. Trojanek[1], P. Nahalkova[1], D. Sprinzl[1], P. Maly[1]
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Chemical bath deposition is one of techniques of fabrication of semiconductor thin films consisting of CdS and CdSe nanocrystals. By changing parameters of preparation, the properties of the films can be modified. In particular, the size of nanocrystals can be tailored, e.g. a single-step nanocrystal-size patterning can be achieved by the modulation of light illuminating the film during the growth. Relaxation and recombination processes of photoexcited carriers in nanocrystals can be studied using techniques of the ultrafast laser spectroscopy. The carrier dynamics is affected not only by their three-dimensional confinement within the nanocrystal volume but also the surface of nanocrystals plays important role. Modification of both the nanocrystal size and the nanocrystal surface makes it possible to optimize the nanocrystalline films for optoelectronic applications.

M4H5    **Ultrafast light-induced magnetization dynamics in III-V ferromagnetic semiconductors**

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We develop a mean field theory of light-induced ultrafast magnetization dynamics in ferromagnetic semiconductors and demonstrate the possibility to control the collective magnetization during sub-picosecond time scals by below-resonant circularly polarized optical pulses. The magnetization dynamics is significantly affected by strong hole spin dephasing.

M4H6    **Ultrafast acoustics**

Emmanuel Péronne[1], Bernard Perrin[1]
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Femtosecond lasers can be used in absorbing media for the excitation and detection of acoustic pulses with a duration of a few ps. These pulses can be used for SONAR experiments in bulk crystals, thin films and multilayers systems or for the excitation of vibrational modes of nano-structures and nano-objects [1]. After a brief discussion of the generation and detection mechanisms and a presentation of a few examples, the processes which limit the acoustic pulses duration above a few ps will be pointed out. However, it has been shown that propagation of picosecond acoustics pulses over large distances in pure crystals at low temperatures allows the formation of acoustic solitons [2,3]. We will describe a recent experimental observation of acoustic solitons using an interferometric detection of the sample surface motion and discuss that evidence of sub-picosecond acoustic pulses can be expected in a very near future.

[1] B. Perrin, in  Systèmes Femtosecondes , P. Laporte and F. Salin (eds.), Publications de lUniversité de Saint Etienne, 2001, 65-89
[2] H. -Y. Hao and H. J. Maris, Phys Rev B **64**, 064302 (2001)
[3] O. L. Muskens, A. V. Akimov, J. L. Dijkhuis, Phys. Rev Lett **92**, 035503/1 (2004)

M4H7 **Time dependant Ferromagnetic Resonance Induced by Femtosecond Optical Pulses in Co films**

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Several ferromagnetic Co thin films, with different magneto-crystalline anisotropies, have been studied in a femtosecond pump probe polarimetric experiment under a static external magnetic field. A detailed study of the magnetisation dynamics reveals the complex trajectory of the magnetization, after excitation with a pump pulse. This trajectory is followed in all three dimensions of the real space. The time resolved polar and longitudinal kerr effect provide the variation of the magnetisation vector in the plane of incidence while the transverse component is obtained from reflectivity measurements. A fast demagnetisation first occurs during a few hundreds of femtoseconds. It is then followed by a precession motion around the effective field . Both the amplitude and period of the precession depend on the pump intensity and the external field.

M4H8 **Time-resolved degenerate four-wave mixing (TR-DFWM) of magneto-excitons in GaAs/AlGaAs single quantum wells (SQW)**

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We have measured the TR-DFWM emission from resonantly-excited excitons in GaAs/AlGaAs SQWs in magnetic fields from 0 to 11T. Single quantum wells of different widths, varying from 5.6nm to 15.0nm are studied with both sigma plus and sigma minus excitation in Faraday geometry. The real-time evolution of the signal shows beating at different frequencies which vary with field, well width, and k1-k2 delay. These beats correspond to the heavy hole/light hole splitting and the spin splitting induced by the magnetic field. Variation of coherence times with magnetic field can be unambiguously extracted from our fully time-resolved data, and make clear the role of state mixing in coherence decay.

*Quantum decoherence and dissipation in mesoscopic system* **Hall J**

M4J1 **Interaction of Josephson qubits with strong QED cavity modes: dynamical entanglement transfer and navigation**

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*1) DMFCI, Universitá di Catania & MATIS - INFM, Catania (I)*
*2) School of Mathematics and Physics, The Queen's University, Belfast (UK)*
*3) DTI, University of Milano, Crema & NEST - INFM, Pisa (I)*
*4) Dipartimento di Fisica, Universitá delle Calabrie, Cosenza (I)*

We study a setup and protocols for information transfer between Josephson qubits, also suitable as a probe of entanglement in the solid state [1]. Interest in the problem also arises from recent proposals of coupling Josephson qubits with solid-state microstrip resonators. We analize in detail decoherence, environment engineering, selection rules, protected subspaces and inhomogeneuos broadening due to 1/f noise.

We then study of entanglement transfer between two remote Josephson qubits mediated by entangled two-mode light fields. We discuss the range of mixed entangled states obtained and a protocol to determine the residual entangling power of the light fields.

M4J2 **The Quantum Smoluchowski Equation**

Joachim Ankerhold[1], Hermann Grabert[1]
*1) Physikalisches Institut, Universitaet Freiburg, Germany*

For a quantum system coupled to heat bath environment the strong friction limit is studied starting from the exact path integral formulation. Generalizing the classical Smoluchowski condition to low temperatures, a time evolution equation for the position distribution is derived, the quantum Smoluchowski equation [1,2]. The substantial role of quantum fluctuations in this limit is discussed. While applications are numerous in physics and chemistry, special attention will be paid to the decay of the zero-voltage state and the relation between quantum phase diffusion and charging effects in overdamped Josephson junctions [3].

[1] J. Ankerhold, H. Grabert, P. Pechukas, Phys. Rev. Lett. 87, 086802 (2001). [2] J. Ankerhold, Europhys. Lett. 61, 301 (2003). [3] J. Ankerhold, cond-mat/0402516.

M4J3 **Tunable Quantum Fluctuations with Josephson SQUID Arrays**

D. B. Haviland[1], W. Guichard[1], S. Corlevi[1]
*1) Nanostructure Physics, Royal Institute of Technology*

We have preformed experiments on Cooper Pair Transistors (CPT), biased through leads consisting of one-dimensional SQUID arrays. These arrays provide a tunable environment, where quantum fluctuations of the variables describing the CPT can be controlled while the DC transport of the CPT is studied. An interesting regime of transport is achieved when the effective impedance shunting the CPT at high frequencies becomes larger than the quantum resistance $R_Q = h/4e^2$. In this case we observe a Coulomb blockade for Cooper pair tunneling in the CPT, with a characteristic threshold voltage for the onset of current, and a sharp back-bending I-V curve. We have studied this Coulomb blockade for various ratios of the Josephson to Charging energies of the CPT. We also observe a modulation of the DC IV curve with gate voltage, and a crossover from 1e to 2e periodic modulation, as the environment is tuned towards higher impedance.

M4J4    **Duality Relation for Quantum Ratchets**

J. Peguiron[1], M. Grifoni[2]
*1) Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands*
*2) Insitute for Theoretical Physics, University of Regensburg, Germany*

We investigate a duality transformation between weak-binding models and tight-binding models for quantum ratchet systems. Ratchets are periodic structures with broken spatial symmetry yielding thepossibility of a directed current in presence of noise and unbiased external forces. The duality allows to relate results that we obtained on few-bands quantum ratchets in the incoherent tunneling regime [1] with existing results on weakly corrugated ratchets [2]. It also makes possible to extend the parameter range of applicability of these results and especially check their classical limit. We are furthermore able to check the spatial symmetry conditions under which the ratchet current vanishes.

[1] M. Grifoni et al., PRL 89, 146801 (2002)
[2] S. Scheidl and V. M. Vinokur, PRB65, 195305 (2002)

M4J5    **Macroscopic quantum effects in a strongly driven nanomechanical resonator**

Michael Thorwart[1], Vittorio Peano[1]
*1) Institut für Theoretische Physik IV, Heinrich-Heine-Universität Düsseldorf*

We investigate the nonlinear response of a vibrating suspended nanomechanical beam on external periodic driving. The amplitude of the fundamental transverse mode behaves thereby like a weakly damped quantum particle in a driven anharmonic potential. Upon using a Born-Markovian master equation, we determine the amplitude of the fundamental mode for varying driving frequencies. In the nonlinear regime, we observe resonances which are absent in the corresponding classical model. They are shown to be associated with resonant multi-phonon excitations. Furthermore, we identify resonant tunneling in the dynamically induced bistable effective potential. The tunneling rate can be alternatively obtained directly from a master equation in the framework of Floquet theory.

# Poster Session 16:00 – 18:00

S4X1 **Electronic and Magnetic Structure of Pu, Am, and Cm**

Andrey L. Kutepov[1]
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In this contribution the calculated electronic structure and magnetic properties of alpha-Pu, delta-Pu, Am, and Cm will be presented. The calculations have been performed with the new full-relativistic full-potential spin-polarized linearized-augmented-plane-wave method (RSPFLAPW)(A. L. Kutepov and S. G. Kutepova, J.Phys.: Condens. Matter 15 (2003) 2607-2624). The effect of taking the magnetic structure into consideration on the calculated ground state properties of the above actinides has been considered.

The electronic systems of the actinides from plutonium onwards are strongly correlated. So, usual approximations (LDA or GGA) are believed to be not very suitable for describing all the properties of these elements. However, the fact, the ground state properties for all the above actinides are described pretty well in GGA when spin polarization is taken into account, makes us think that some correlation effects which are important for obtaining the equilibrium properties for these elements are already contained in this approach.

S4X2 **SUM RULES FOR FOUR-SPINON DYNAMIC STRUCTURE FUNCTION IN ANTIFERROMAGNETIC HEISENBERG MODEL**

Abdessamad Abada[1], Bahia Si-Lakhal[2]
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*2) Département de Physique, Université de Blida, BP 270 Blida 09000, Algeria*

Sum rules are calculated for the exact four-spinon dynamic structure function (DSF) $S_4$ in the antiferromagnetic spin 1/2 Heisenberg quantum spin chain. These sum rules are known to be exactly satisfied by the total DSF $S$. Hence, it is possible to measure and discuss by how much $S_4$ corrects the contribution from the dominant two-spinon DSF $S_2$ to the total $S$. The sum rules involve multiple integrals which are handled using Monte Carlo methods. Statistics and precision are discussed.

S4X3 **Resonance peak and incommensurability in cuprate perovskites**

A. Sherman[1], M. Schreiber[2]
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*2) Institut für Physik, Technische Universität, D-09107 Chemnitz, Germany*

The magnetic susceptibility of underdoped cuprates is interpreted based on the self-consistent solution of the $t$-$J$ model. The calculations reproduce correctly the frequency and momentum dependencies of the resonance peak in YBCO, its variation with doping and temperature in normal and superconducting states. The peak frequency $\omega_{\mathbf{Q}} \approx 20 - 40$ meV is determined by the spin gap at $\mathbf{Q} = (\pi, \pi)$. The low-frequency shoulder of the peak is related to the nesting of the hole Fermi surface. For $\omega \ll \omega_{\mathbf{Q}}$ the susceptibility is peaked at incommensurate wave vectors $(\pi \pm 2\pi\delta, \pi)$, $(\pi, \pi \pm 2\pi\delta)$. The incommensurability is connected with the minimum in the magnon damping at $\mathbf{Q}$ in a crystal with the short-range antiferromagnetic order. In agreement with experiment $\delta \propto x$ for hole concentrations $0.02 < x \leq 0.12$ and saturates for larger $x$. Generally the incommensurability is not accompanied by an inhomogeneity of the carrier density.

S4X4 **Orbital ordering in B-site doped manganites**

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We have measured the reflectivity spectra of $La_{1-x}[Sr(Ba)]_x Mn_{1-z}[Cu(Zn)]_z O_3$ ($0.17 \leq x \leq 0.3$, $0 \leq z \leq 0.10$) manganites in a wide frequency and temperature range. Besides previously observed infrared active modes or mode pairs at about 160 cm$^{-1}$ (external mode), 350 cm$^{-1}$ (bond bending mode) and 590 cm$^{-1}$ (bond stretching mode), we have clearly observed two additional phonon modes at about 645 cm$^{-1}$ and 720 cm$^{-1}$ at a temperature $T_1$ ($<T_C$), which coincides with the phase transition temperature when the system transforms from ferromagnetic metallic into ferromagnetic insulator state. Electrical resistivity and magnetization measurements vs temperature and magnetic field support the orbital ordering scenario.

S4X5 **Inhomogeneous Ferromagnetic ground state in Ce alloys studied by magnetocaloric effect**

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We present the study of heat capacity in fields up to 9T and temperature down to 500 mK in some FM representative compositions of the pseudobinary $CeNi_{1-x}Cu_x$ alloys : x = 0.6, 0.5, 0.4 and 0.2.
In spite of the very small effective magnetic moment of Ce the observed magnetocaloric effect is moderately high.This result is discussed according to previous results obtained in these series, taking into account the cluster model proposed in this system .

S4X6 **Oxide half-metals**

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We will present tunnel magnetoresistance results on junctions integrating one or two $La_{2/3}Sr_{1/3}MnO_3$ (LSMO) electrodes. We will show that this compound has a spin-polarization of more than 95% at low-temperature and present results on LSMO-based junctions integrating different barrier materials ($SrTiO_3$, $LaAlO_3$, $TiO_2$, $Al_2O_3$) and counter-electrodes ($Co_{1-x}Cr_x$), from which an analysis of the fundamental mechanisms of spin-polarized tunneling can be performed. Another material for which a half-metallic character has been predicted by band-structure calculations is the $Sr_2FeMoO_6$ double perovskite. We have fabricated tunnel junctions with this material and we will show that it has a negative spin-polarization of about 90% at low-temperature.

S4X7 **Magnetism of 4f ferromagnetic insulators**

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Using mapping of the ab initio groundstate energies obtained with LDA+U method onto Heisenberg Hamiltonian we have calculated the effective exchange parameters and ordering temperatures of members of the europium chalcogenide series. The trend accross the series as well as the pressure dependences of the ordering temperatures compare well to the experimental data. Analyzing the impact of different choices of U we arrive at some conclusions about the coupling mechanisms involved. Our results demostrate the ability of the LDA+U method to describe accurately exchange interactions in materials with localized moments and suggest LDA+U electronic structure to be a sound basis for further computational investigation of mechanisms of inter-site exchange coupling.

S4X8 **Quasi-Particle Dispersion Relation for a Ferromagnet near a Quantum Critical Point**

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The effect of ferromagnetic spin-fluctuations on the quasi-particle dispersion relation is examined for a ferromagnet near a quantum critical point. The spin-fluctuations in a ferromagnet can be divided into two contributions, the branch of Goldstone modes which satisfy the dispersion relation $\omega = Dq^2$, and a Stoner continuum consisting of $S = 1$ electron-hole pair excitations. The Stoner continuum exhibits a $q = 0$ threshold (the exchange-splitting). It is found that the spin-fluctuations produce a large frequency-dependent self-energy which renormalizes the quasi-particle mass and the exchange-splitting. It is found that that the main contribution to the renormalization arises from the incoherent excitations of the ferromagnet, in a manner similar to the incoherent excitations on the paramagnetic side of the quantum critical point. The ineffectiveness of the Goldstone modes can be understood in terms of their role of dynamically restoring the spontaneously broken symmetry of the ordered state.

S4X9 **The peculiarities of conductivity and termopower in a model of doped Mott-Hubbard material**

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In this work the peculiarities of static conductivity and termopower in a model of doped Mott-Hubbard material with strong intra-atomic electron interactions are investigated theoretically. The static conductivity has been calculated at arbitrary temperatures within a projection procedure in Green function technique. The expressions for conductivity and termopower in lower and upper Hubbard subbands are found as functions of temperature, strain of the lattice (dependent on the pressure), electron concentration and parameters of correlated hopping of electrons. The conductivity and termopower are shown to depend strongly on doping and temperature. The obtained dependencies allow to interpret the experimental data for electrical conductivity in a static field and termopower of transition metal compounds in which electron-hole asymmetry is observed.

S4X10 **Magnetization and specific-heat study of UCoAl$_{0.75}$Sn$_{0.25}$**

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The UCoAl$_{0.75}$Sn$_{0.25}$ single crystal has been grown and studied by measuring the magnetization and specific heat. Similar to the parent compounds, the band metamagnet UCoAl and the ferromagnet UCoSn, the magnetization of UCoAl$_{0.75}$Sn$_{0.25}$ exhibits the uniaxial anisotropy with a strong magnetic response along the $c$ axis and a weak and nearly temperature independent paramagnetic signal in the basal plane. Evolution of the $c$ axis magnetization isotherms, as well as the anomalies in the temperature dependence of the specific heat point to ferromagnetism in UCoAl$_{0.75}$Sn$_{0.25}$ below $T_C$ = 5.5 K. The low value of spontaneous magnetic moment, poor saturation of the magnetization and the temperature and magnetic field dependence of specific heat provide indications of strong fluctuations of the U magnetic moment also in the ferromagnetic state.

S4X11 **Orbital Anisotropy and Geometrical Frustration in Strongly Correlated Electron Systems**

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We investigate the $e_{\mathrm{g}}$-orbital degenerate Hubbard model at quarter filling on the zigzag chain and the ladder, by using the density matrix renormalization group method. In the ladder, the spin correlation on the rung remains robust due to the absence of frustration, while in the zigzag chain, the system is effectively regarded as a double chain of the $S$=1/2 antiferromagnetic Heisenberg chain, since the spin correlation between two chains is weakened due to spatial anisotropy of $e_{\mathrm{g}}$ orbital to suppress the effect of frustration. For the zigzag chain, we also investigate the effect of the crystal-field splitting between energy levels of $3z^2-r^2$ and $x^2-y^2$ orbitals, which suppresses orbital degree of freedom and revives geometrical frustration.

S4X12 **$^{59}$Co-NMR studies of Na$_{0.70}$CoO$_2$**

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We have performed $^{59}$Co-NMR measurements on polycrystalline samples of Na$_{0.7}$CoO$_2$ at temperatures between 0.1 and 300 K. Below 200 K, the spin lattice relaxation rate $T_1^{-1}$ varies linearly with temperature and between 30 and 300 K the Knight shift is temperature independent. These results are characteristic for nonmagnetic nuclei in a metallic environment. They show that the CoO$_6$ planes of Na$_{0.7}$CoO$_2$ are metallic and, considering the results for the magnetic susceptibility, one may conclude that below 200 K, only part of the Co ions carry a magnetic moment. The $^{59}$Co-NMR response is very different from the $^{23}$Na-NMR response. The latter shows that, as expected, the basal Na planes are insulating. Above 200 K the $^{59}$Co-$T_1^{-1}$ substantially increases above the values expected from the low-temperature linear-in-$T$ behavior. This increase adds support to our previous claim of a dramatic change in the Co 3$d$-electron spin dynamics below 300 K.

S4X13 **Elastic property of filled skutterudite compounds SmRu4P12 and CeOs4Sb12**

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We measured elastic constants and sound attenuation on filled skutterudite compounds SmRu4P12 and CeOs4Sb12. A remarkable anomaly was observed in elastic constants and attenuation at 16 K accompanied by metal-insulator transition. We will discuss the 4f-ground state of Sm ion and the nature of transition from the standpoint of the quadrupolar moment. On the other hand, a pronounced softening toward low temperatures was observed in C11 in kondo-semiconductor CeOs4Sb12.The origin of this softening will be discussed based on the coupling between enhanced carriers by hybridization and a relevant elastic strain induced by sound wave.

S4X14 **Kondo effect behaviors in the Gd-based inter-metallic compound**

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X-ray diffraction, electrical resistivity and magnetic susceptibility measurements of Gd-based inter-metallic compound (Gd2 Al(1-x) Aux ), prepared by a standard Arc-melting furnace are investigated. The spectrum of X-ray diffraction revealed an orthorhombic crystal structure with the pnma space group (all the samples are iso-structural). We observe a strong deviation from Vegards rule and a sharp variation of the unit cell volume (6 per cent) at the critical point x = 0.4. It is found that the value of the susceptibility shows a decrease and we have observed an increase in Tc (Curi temperature) with increasing x. For the compound with x = 0.4 the electrical resistivity shows a minimum at about 70 K . The observed behavior in this compound (necessary for the Kondo behavior) could be explained by the presence of a virtual band state from a localization of the conduction electron via due to an exchange interaction (s-f), forming a canted system. For the compound x =0.4 there is a weak increase (3per cent) of the resistance below 70 K. This anomalies could be explain by the formation of an antiferromagnetic phase as a second phase existing in presence of the ferromagnetic phase. The double phase coexistence in this system can attribute to the formation of the canted behavior of the virtual band state. We carry out the measurements of susceptibility in function of the temperature in low and high magnetic fields.

S4X15 **Quantum Hall Physics in Noncommutative Manifold**

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The first quantized system of particles in a strong magnetic field naturally realizes a noncommutative space. When the electron density lies at certain rational fractions of the density corresponding to the fully filled Landau level, the electrons condense into an incompressible fluid-like states whose excitations are characterized by fractional charges and are described by Laughlin wave functions. Taking resort to Haldane's spherical geometry we can visualize fractional quantum Hall effect on the noncommutative manifold such that the discrete space leads to the deformation of symplectic structure of the continuous manifold. We here argue that this is equivalent to the noncommutative field theory as prescribed by Susskind and Polychronakos which is characterized by area preserving diffeomorphism. The filling factor 1/m is determined from the change in chiral anomaly and hence the Berry phase as envisaged by the star product.

S4X16 **Exact solution of the Lai-Sutherland model with a random walk magnetic impurity**

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We study particular type of a magnetic impurity in the Lai-Sutherland chain by means of the Bethe ansatz method. The transport mass of an impurity is equal to zero, in contrast with itinerant electrons the impurity random walks do to scattering electrons on the impurity. It was found that the behavior of the impurity is characterized by the Kondo temperature at a strong coupling limit, the value of that depends on the band filling. In contrast with the Kondo problem the local moment of impurity has not crossover from a linear behavior for small fields to a constant value at large magnetic fields. We shown that depending on the external magnetic field and the density of electrons, the local moment of impurity can either be totally screened, partially screened or overscreened. The overscreening of the local moment is realized at high electron density when itinerant electrons on nearest-neighbor lattice sites screen the impurity.

S4X17 **Ultrasonic investigation of $(La_{0.4}Pr_{0.6})_{1.2}Sr_{1.8}Mn_2O_7$ in pulsed magnetic field**

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We have measured the sound velocity change and ultrasonic attenuation of a Pr-doped layered manganite $(La_{0.4}Pr_{0.6})_{1.2}Sr_{1.8}Mn_2O_7$ in the pulsed magnetic field. Pulsed magnet provides the maximum field of 35 T in 7 msec. We can obtain approx. 200 data in one field scan by a specially-tuned hand-made ultrasonic apparatus. This material undergoes a field-induced insulator-to-metal (I-M) transition at low temperatures. Sound velocity and ultrasonic attenuation show interesting field dependence associated with I-M transition and even in metallic phase. We will discuss these results acquired in very short time scale, by comparing to those carried out in stationary field.

S4X18 **TRANSPORT AND THERMODYNAMIC PROPERTIES OF $Na_xCoO_2$**

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Electronic transport in the layered $Na_xCoO_2$ (x=0.65, 0.7, 0.75) has been investigated in the temperature range of 3-360K and magnetic field up to 14T. Correspondence with the previous specific heat and susceptibility data was found, indicating a magnetic phase transition at 28 K and anomalies around 250 K that can be associated to charge ordering.

**S4X19** **Exchange interactions in the molecular nanomagnet Mn12**

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We perform inelastic neutron scattering measurements on the molecular nanomagnet Mn12-acetate to probe magnetic excitations. They are found between 5 and 10.5 meV, with higher levels appearing only at 27 meV and 31 meV. We show that all of the low-energy modes appear to be $S = 9$ excitations above the $S = 10$ ground state, with the peak at 27 meV being the first $S = 11$ excitation. A general model for the four exchange interaction parameters of the molecule is considered. The theoretical results (high-T series expansion and exact diagonalization) are compared to experimental observations. Only a model with dominant exchange couplings $J1 \sim J2 \sim 5.5$ meV and small couplings $J3 \sim J4 \sim 0.6$ meV is consistent with experiments.

**S4X20** **Variational optimized approach for electron-phonon problems**

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The interaction of electrons with local lattice deformations plays an important role in many different materials leading to a number of effects that range from colossal magnetoresistance in manganites to superconductivity in fullerenes, from pseudo- gap in cuprates to Peierls instability in quasi one dimensional materials. By using a variational approach based on expansion in coherent states, we present the numerical data on small clusters for the extended Holstein model. It is shown that different types of lattice distortions are present at intermediate electron-phonon coupling as observed in cuprates and manganites.

**S4X21** **Fermi Surface and Band Structure of UGe$_2$**

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UGe$_2$ is of high current interest due to the possible role of FM fluctuations in its pressure induced superconductivity. The band structure and Fermi surface contours of a single crystal have been measured using resonant ARPES near the U $5d$ to $5f$ edge. Detailed comparison is made to ThGe$_2$ LDA UGe$_2$ LDA+U band calculations. The measured dominant large sheet FS contour shows agreement with dHvA frequencies, and contains a simple diamond-like shape that is suggestive of a possible diagonal nesting condition different than previously proposed for SCDW models of the FM transition(s) in UGe$_2$.

S4X22 **YbIr$_2$Si$_2$: Fermi liquid homologue of the non Fermi liquid YbRh$_2$Si$_2$**

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YbIr$_2$Si$_2$ ($T_N$ = 70 mK) has been intensively investigated due to its proximity to a quantum phase transition. We have investigated high quality single crystals (RRR > 200) of the related compound YbIr$_2$Si$_2$. Depending on synthesis conditions the samples take either body-centred (I-type) or primitive (P-type) tetragonal structure. P-type sample shows AF order below 700 mK. I-type sample is a heavy fermion ($\gamma$ = 0.37 J/mol K$^2$) and does not show any signature of magnetic or superconducting transition down to 20 mK. The temperature dependence of resistivity shows a behavior typical of Kondo lattice systems. Below 200 mK a quadratic decrease of the resitivity with T and a constant Sommerfeld coefficient C/T evidence Fermi-Liquid behavior. The absence of magnetic transition and the Fermi-liquid behavior indicate that I-type YbIr$_2$Si$_2$ is located on the non-magnetic side of the quantum critical point (QCP), in contrast to YbRh$_2$Si$_2$. Thus, YbIr$_2$Si$_2$ is suitable system to investigate pressure induced quantum phase transition.

S4X23 **Magnetism in CePt$_3$X ( X = B, Al, Si and Ge) Compounds**

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A series of isostructural CePt$_3$X intermetallics (X = Si, Al, Ge, B) has been synthesized and characterized by X-ray powder diffraction and microprobe analysis. All compounds crystallize in the non-centrosymmetric CePt$_3$B type structure with a space group P 4mm. CePt$_3$Si is the first known heavy fermion superconductor without symmetry center with AF ordering below $T_N$ = 2.2 K followed by a SC transition at $T_C$ = 0.75 K. The specific heat and resistivity dependencies of CePt$_3$Al and CePt$_3$Ge show several anomalies in the low temperature region (below 4K), while the specific heat of CePt$_3$B exhibits three anomalies, at 6.8 ($T_N$) K, 4.9 K ($T_C$) and 1.8 K, respectively. No sign of superconductivity has been observed down to 0.35 K for CePt$_3$Al, CePt$_3$Ge and CePt$_3$B, respectively.

S4X24 **Asymmetric Hubbard Model in Dynamical Mean-Field Approximation**

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An approximate analytical scheme of the dynamical mean-field theory (DMFT) is developed for the description of electron (ion) systems with Hubbard correlations within the asymmetric Hubbard model where the chemical potentials and electron transfer parameters depend on the electron spin (sort of ions). The effective single-site problem is formulated in terms of the auxiliary Fermi-field. A system of DMFT equations is obtained in the generalized Hubbard-III approximation. The approximation is tested on the infinite-$U$ spinless Falicov-Kimball model. The densities of states of electrons and localized particles are obtained at various particle concentrations and temperatures. Dependences of energy band edges and chemical potentials on concentrations are analyzed at finite repulsion $U$ and different values of asymmetric transfer parameters within the Hubbard-I and alloy-analogy approximations in the different thermodynamic regimes.

S4X25 **DMFT treatment of Raman scattering in strongly-correlated materials.**

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We investigate the electronic Raman scattering in strongly correlated materials via dynamical mean field theory. The nonresonant, resonant and mixed contributions to Raman responce function for all the symmetry channels are calculated exactly for the spinless Falicov-Kimbal model. We obtain significant enhancement of nonresonant scattering peaks due to the resonance. The appearance of an isosbestic point and a triple resonance peak as well as the joint resonance of the charge transfer and low energy peaks are the other important features.

S4X26 **Magnetism and superconductivity in $CeCu_2(Si_{1-x}Ge_x)_2$**

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The heavy fermion system $CeCu_2(Si,Ge)_2$ is of high interest because of the interplay between heavy - fermion superconductivity and magnetism. An extensive microscopic study has been prevented by the absence of large single crystals. We used a modified Bridgman technique with Cu excess as flux and grow large single crystals. We were able to detect magnetic reflexes with neutron scattering. For x = 0.45 we found an incommensurate antiferromagnetic order with a propagation vector $\tau$ = (0.28, 0.28, 0.51) and an ordered moment of 0.5 $\mu_B$. Upon decreasing the Ge-content, we observed only a slight change of the propagation vector, while the size of the ordered magnetic moment strongly decreases. Analysis of thermodynamic and transport properties indicate the transition from an antiferromagnetic state of local moments at higher Ge-contents (x > 0.25) to a spin density wave of itinerant heavy fermions at lower Ge contents (x < 0.25).

S4X27 **XANES study of Mn and Co valence state in LaMn1-xCoxO3**

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A XANES study of LaMn1-xCoxO3 perovskites is reported. Measurements at the Mn, Co: K, L2, L3 and O: K edges have been carried out for samples with x = 0.2; 0.4; 0.6; 0.8 and 1.0. The L2,3-edges of manganese reveal a systematic change with x and could be reproduced by linear combination of reference spectra of MnO2 (Mn4+) and Mn2O3 (Mn3+). The K-edges of Mn and Co show a gradual shift to higher energies with increasing x which also indicates the existence of mixed states Mn3+/Mn4+ and Co2+/Co3+ in doped samples and is consistent with the evolution of the oxygen K-edge spectra. The relation to the magnetic and transport properties of the compounds is discussed.

S4X28 **Quantum spin state mixing in frustrated nanomagnets**

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The molecular spin cluster V15 is a polyoxovanadate with 15 spins s=1/2 but total spin ground state S=1/2 due to strong antiferromagnetic (AFM) interactions. The ground state is composed of two non-degenerate S=1/2 Kramers doublets separated by a gap of about 0.3 K. The mechanism leading to such gap formation in the ground state has been elucidated using inelastic neutrons scattering (INS) under magnetic field. The observation and characterisation of several field-dependent INS transitions enable a comprehensive understanding of the low-energy quantum spin states including a quantitative description of the wavefunction mixing within the ground state.

S4X29 **Pressure effect on multiple metamagnetic transitions in $Sr_3Ru_2O_7$.**

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$Sr_3Ru_2O_7$ is a $4d$-electron metamagnet showing pronounced non-Fermi liquid behavior, which can be tuned by magnetic field. Magnetization curve of the compound has several S-shaped anomalies (2 or 3 depending on the field direction) instead of a single transition expected for an itinerant electron metamagnet (IEM). The corresponding induced high-magnetization states of $Sr_3Ru_2O_7$ survive the application of at least 1.2 GPa hydrostatic pressure although the critical fields separating them, $H_{c1}$ and $H_{c2}$, have different character of pressure dependence. The increase of $H_{c1}$ and $H_{c2}$ with increasing pressure cannot be accounted for by the classical IEM theory. It may suggest that the first metamagnetic transition produces an unstable magnetic structure with large entropy, which is then stabilized by subsequent metamagnetic transitions.

S4X30 **Novel diluted magnetic semiconductors $Sb_{2-x}V_xTe_3$ and $Sb_{2-y}Cr_yTe_3$**

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We report on novel diluted magnetic semiconductor based on the $Sb_2Te_3$ tetradymite structure. $Sb_{2-x}V_xTe_3$ (x=0.0-0.03) and $Sb_{2-y}Cr_yTe_3$ (y=0.0-0.095) single crystals were prepared from the elements Sb, V, Cr, and Te of 5N purity by a modified Bridgman method. The obtained crystals were characterized by measurements of the temperature dependence of the electrical resistivity, Hall coefficient, and magnetic susceptibility in the temperature range of 2-300 K. It was observed that a small content of vanadium in the $Sb_2Te_3$ crystals gives rise to ferromagnetic behavior at low temperatures, the Curie temperature $T_C$ increases with vanadium content and reaches approximately 22 K for $Sb_{1.97}V_{0.03}Te_3$. Above $T_C$, the temperature dependences of magnetic susceptibility are well fitted by a Curie-Weiss law, the values of the effective Bohr magneton number per vanadium atom $p_{eff}$ increase from 1.9 to 2.6 as x increases from 0.01 to 0.03. This might indicate an evolution to a predominantly 3+ valence state of vanadium (expected spin only value of $p_{eff} = 2.83$). Single crystals of $Sb_{2-y}Cr_yTe_3$ for y≥0.031 are ferromagnetic, with Curie temperatures that depend linearly on Cr content, a maximum value of $T_C$ is 20 K for y=0.095. Magnetic as well as transport data indicate that Cr atom takes the 3+ valence state, substituting for antimony in the host lattice structure, and does not significantly affect the background hole concentration. The research was supported by Ministry of Education of Czech Republic under the project KONTAKT ME 513 and the NSF grant INT 0201114.

S4X31 **MBE growth and characterization
of EuGdTe ferromagnetic semiconductor**

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EuGdTe ferromagnetic semiconductor is expected to be useful for injection of spin polarized charge carriers into non-magnetic semiconductor. Ferromagnetic ordering in this material results from $Gd^{3+}$ (substituting $Eu^{2+}$) conducting electrons, what induces RKKY interaction between spins localized on both magnetic ions. We report growth of n-type EuGdTe epitaxial layers with Gd content up to 5%, grown in home-built MBE machine. The samples were characterized *in situ* using RHEED revealing well defined streaky two-dimensional patterns and *ex situ* by XRD and AFM studies. The temperature dependence of magnetic susceptibility shows transition to ferromagnetic ordering near $T_C$=13 K. Correlated behavior in resistivity vs temperature, due to scattering of carriers on the giant spin moment while temperature is lowered to $T_C$, is also observed.

S4X32 **Generalized mean-field theory of semiconductors and metals with magnetic impurities**

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*Random* systems of magnetic moments positioned in cites of a crystal lattice and interacting via RKKY- or Bloembergen–Rowland-type interaction are considered in the framework of *generalized* mean-field theory (GMFT) based on calculating and analyzing *distribution functions* $F(H)$ of random *local* magnetic fields $H$. For *concentrated* systems (where the random local field is produced by a number of interacting magnetic moments), the function $F(H)$ turns out to be Gaussian one and all information about the system is contained in two parameters of that distribution only – its width and maximum position. For *rarefied* systems (where the average distance between interacting moments is comparable with or larger than the interaction length), distribution functions are essentially non-Gaussian. GMFT has been applied for calculating the magnetic state of metals and semiconductors diluted with magnetic impurities.

S4X33 **Spin Waves in Diluted-Magnetic-Semiconductor Quantum Wells**

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We present a theory of collective spin excitations in diluted magnetic semiconductor quantum wells, in which local magnetic moments are coupled via a quasi-two-dimensional electron or hole gas. In contrast to bulk systems, a multiplet of spin-wave branches is predicted. We discuss the dispersion of these collective excitations and the profiles of the corresponding modes for different magnetic-ion doping concentrations and free-carrier densities. In the case of a ferromagnetic state with a partially spin-polarized two-dimensional electron gas, we find that the Goldstone collective mode has anomalous $k^4$ dispersion and that for symmetric quantum wells odd parity modes do not disperse at all. Moreover, we further discuss the gap in the collective excitation spectrum which appears when spin-orbit interactions are included. [cond-mat/0312347, to appear in Phys. Rev. B].

S4X34　**Oxidation of thin tilms of TaSi$_2$ and WSi$_2$ prepared on polycrystalline Si**

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XPS and UPS have been used for studying the oxidation of TaSi$_2$ and WSi$_2$ thin films formed by annealing of metal deposits ($\sim$70$\overset{\circ}{A}$) of on polycrystalline Si. Oxidation has been carried out at room temperature and at 700 $^o$C with an oxygen pressure of the 2x10$^{-5}$ mbar. For WSi$_2$, SiO$_2$ oxide is on surface. W atoms did not oxidize. The electronic structure and stoechiometric composition of WSi$_2$ is preserved. For TaSi$_2$ layer, at room temperature both Ta and O react with oxygen. O chemisorbs on the surface giving a mixed phase of Si suboxide and Ta oxides. At 700 $^o$C, a very thin Ta$_2$O$_5$ layer is formed on the top of the growing SiO$_2$ layer. In comparison with Si (111) the oxidation kinetics of TaSi$_2$ and WSi$_2$ begin with higher transitory rate and follows afterwards the same parabolic dependence of the SiO$_2$ thickness as a function of oxidation time. Oxidation mechanism proposed is: oxidation takes place at the Si oxide-Silicide interface and oxygen diffusion through SiO$_2$ is the rate-limiting step in the oxidation process.

S4X35　**Theory of magnetotransport in magnetic semiconductors and hybrid structures**

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We study theoretically the magneto-transport in paramagnetic semiconductors and paramagnetic-ferromagnetic hybrids. A resistor network based on a minimal description of the band structure of the DMS is developed. Band filling effects, magnetic-field splitting of the band states due to the p-d exchange interaction, effects of magnetic-field independent disorder and of the ferromagnetic clusters are included whereas carrier-carrier interactions other than those responsible for the local magnetism of the Mn ions are neglected. Despite the exclusion of many-body effects in the bands, positive and negative MR effects are predicted for paramagnetic semiconductors in qualitative agreement with recent experiments. Experimentally, the MR behavior of paramagnetic semiconductors and corresponding paramagnetic-ferromagnetic hybrid structures differs considerably. First theoretical descriptions of these differences are presented.

S4X36　**Magnetotransport in GaMnAs/MnAs paramagnetic-ferromagnetic hybrids**

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Hybrid semiconductor-ferromagnet structures based on III-V compounds exhibit high Curie temperatures and tuneable magnetic interactions. We have performed magnetotransport on p-type (GaMn)As/MnAs paramagnetic-ferromagnetic hybrids prepared by MOVPE. The samples exhibit a negative MR (-30%) at low temperatures and with increasing temperature the MR becomes positive with values up to about 160% at H=10 T. In addition, a variation of the Hall constant with magnetic field is observed, which indicates a spin accumulation of carriers in the vicinity of the clusters. These carriers are gradually released when the magnetic field is increased. Both the MR and Hall effect depend strongly on cluster size, temperature and transport geometry. The interaction between ferromagnetic MnAs clusters and the carriers in the paramagnetic (Ga,Mn)As matrix plays an important role in the magnetotransport of these hybrids.

S4X37 **Magnetic properties of diluted magnetic semiconductors $Pb_{1-x}Ge_xTe$:Cr**

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To establish connection between magnetic properties and electronic structure the magnetic susceptibility (T=4.2-300 K, B¡0.5 T) of the diluted magnetic semiconductors $Pb_{1-x}Ge_xTe$:Cr (x=0.02-0.06, $C_{Cr}\sim0.3$ mol.%) was studied. It was found that at low temperatures magnetic susceptibility versus temperature dependences contain paramagnetic Curie contribution. However, the additional ferromagnetic contributions of unknown nature on the temperature and the field dependences of magnetic susceptibility were revealed.Temperature dependencies of the reverse magnetic susceptibility were used to determine the magnetic ion concentration, which monotonously grows with the increase of germanium content. Obtained experimental results were discussed in the frame of the model assuming the formation of magnetically active $Cr^{3+}$ ions and existence of deep chromium impurity level in the energy spectrum of the alloys.

S4X38 **Ferromagnetic exchange coupling in n-type doped (Ga,Mn)As**

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Ferromagnetic exchange interaction in (Ga,Mn)As is generally believed to be mediated by itinerant holes in the valence band and restricted to the p-type materials. We use a tight binding version of the coherent potential approximation to describe the electronic structure of $Ga_{1-x}Mn_xAs$ mixed crystals with variable degree of co-doping and to estimate the exchange coupling from the energy $E_{rev}$ required to reverse one local moment. We found that the dependence of $E_{rev}$ ($\propto T_c$) on carrier concentration $n$ scales as $E_{rev}/x = F(n/x)$. The exchange is antiferromagnetic in compensated materials. It changes to ferromagnetic whenever the number of either holes or conduction electrons exceeds $\approx x/4$ and saturates at $|n| \approx x$. The electron-mediated ferromagnetism is explained as a result of a disorder-induced reconstruction of the conduction band, that makes possible its hybridization with Mn d-states.

S4X39 **Low Temperature Magnetoresistance of (Zn,Co)O Films**

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We have carried out milikelvin magnetoresistance (MR) studies of diluted magnetic semiconductor (Zn,Co)O. Our results demonstrate the existence of a low-field, strongly temperature dependent positive MR and a high-field negative MR. By a comparison of the results with theory that takes quantum correction to the conductivity into account we find that the positive component is caused by the effect of the spin-splitting on disorder-mediated electron-electron interactions, whereas weak localization accounts for the negative MR. We conclude that transport properties of the film are controlled only by the paramagnetic contribution to total magnetization.

S4X40 **Carrier-induced ferromagnetism in the nitrogen doped diluted magnetic semiconductor Zn1-xMnxSe**

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A systematic study of the ferromagnetic transition induced by the holes in nitrogen doped Zn1-xMnxSe epitaxial layers is performed. We have given particular emphasis on the values of the Curie-Weiss temperature as a function of the carrier and spin concentrations. The data are obtained from the analysis of the results of magnetization, magnetoresistance and spin-dependent Hall effect measurements. The experimental finding agrees well, without adjustable parameters, with the prediction of the Rudermann-Kittel-Kasuya-Yosida (RKKY) model or its continuous-medium limit, that is, the Zener model. At the same time the presence of the competing antiferromagnetic spin-spin superexchange interaction is taken into account. The complex structure of the valence band is properly incorporated into the calculation of the spin susceptibility of the hole liquid. As an outcome of our systematic study, the findings demonstrate how the interplay between the ferromagnetic RKKY interaction, carrier localization, and intrinsic antiferromagnetic superexchange affects the ordering temperature and the saturation value of magnetization in magnetically and electrostatically disordered systems.

S4X41 **Electrical and magnetic properties of neutron-irradiated polycrystalline Ge1-xMnx semiconductors grown by MBE**

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MBE-grown Ge1-xMnx semiconductors were irradiated by fast neutrons of 0.82 MeV. Irradiation rate was 3.45x10E10 n/cm2sec and the irradiations were 2.4x10E14, 10E15, 10E16 and 10E17 n/cm2, respectively. Majority carriers are p-type and it does not changed by neutron irradiation. Carrier concentration and mobility decrease with neutron irradiation. Saturation magnetization measured at 2K-300K decreases with neutron irradiation. But the coercive force of Ge1-xMnx semiconductors increases with neutron irradiation. XRD analysis shows that phase transformation is not developed by neutron irradiation. It consideded that formation of point defects, such as self-vacancy and self-interstitals, is responsible for the change of the electrical and magnetic properties.

S4X42 **Anisotropic RKKY interactions in (Ga,Mn)As**

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It is generally agreed that ferromagnetism in diluted magnetic semiconductors is due to magnetic interaction between impurity spins mediated by charge carriers, although there is no complete agreement on the detailed mechanism. We report on a study of the hole-impurity exchange interaction and the RKKY interaction between Mn spins in (Ga,Mn)As based on a model that accounts realistically for Coulomb correlations on the Mn site and hybridization between Mn d and As p orbitals. We use this model to discuss the character of the RKKY interactions and the range of applicability of the RKKY picture of magnetic interactions. We find that the interraction is highly anisotropic both in real space (i.e., the interaction between two spins depends on the direction of the separation vector) and in spin space (i.e., the exchange interaction is described by a matrix in spin space that it not proportional to the unit matrix).

S4X43 **Electrical and magnetic properties of Cr-doped ZnO thin films grown by reactive magnetron sputtering**

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We report on the electrical and magnetic properties of Cr-doped ZnO ($Zn_{1-x}Cr_xO$) and Cr, Al codoped ZnO ($Zn_{1-x}Cr_xO$:Al) films grown by reactive sputtering. The solubility limit of Cr in ZnO is as low as about 0.01 at an optimum growth condition. Magnetic measurements show a weak ferromagnetic characteristic at 5 K for the $Zn_{0.09}Cr_{0.01}O$ films. By Al doping, the injection of $n$-type carrier is achieved and the magnetic properties drastically change, exhibiting a remarkable increase of the saturation magnetization. These results show carrier-enhanced ferromagnetic order in Cr-doped ZnO.

S4X44 **Modified magnetic properties of (II,Mn)VI in nanowires**

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Arrays of (II,Mn)VI quantum wires with diameters below 10 nm and Mn contents $x$ between 0% and 100% are synthesized by incorporating (II,Mn)VI into mesoporous $SiO_2$. Quantum confinement effects of up about 200 meV were observed in the narrowest wires. An increased band-gap bowing versus $x$ occurs in the (Cd,Mn)S wires compared to bulk. A reduced macroscopic antiferromagnetic coupling between the $Mn^{2+}$ ions is found in the wires. For $x > 0.8$, a suppression of the paramagnetic to antiferromagnetic phase transition of the Mn system is observed for the 3 nm wires. For 6 and 9 nm wires a phase transition occurs, but the Néel temperatures are smaller than in bulk. The observed behavior yields information about the length scale of the antiferromagnetic ordering.

S4X45 **Optimisation of Co-doped $La_{0.5}Sr_{0.5}TiO_3$ epitaxial thin films**

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Recent experiments have shown Co-doped:$La_{0.5}Sr_{0.5}TiO_3$ (LSTO) as a diluted magnetic system with a high $T_C$ (APL 83, 2199). $La_{0.5}Sr_{0.5}TiO_3$:Co(1.5%) layers were grown by PLD on $SrTiO_3$(100) at $O_2$ pressures (P) ranging from $6\ 10^{-7}$ to $2.3\ 10^{-4}$ mbar. All the films are epitaxial and ferromagnetic ($T_C > 300$ K). Upon decreasing P the out of plane cell parameter decreases and the electrical conductivity increases while the magnetization shows a maximum (2.38 $\mu_B$/Co) at P $= 5.1\ 10^{-6}$ mbar. Experiments are being carried out to determine the origin of ferromagnetism and to measure the carriers' spin-polarization.

## S4X46 **Anomalous Hall Effect in narrow gap ferromagnetic semiconductors**

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The aim of our work was to study Anomalous Hall Effect (AHE) in narrow gap ferromagnetic semiconductors. We studied transport and magnetic properties of IV-VI compounds: SnMnTe, SnMnEuTe, SnMnErTe, as well as InMnSb – a member of III-V group. Investigations were performed in static magnetic fields up to 13 T and pulsed magnetic fields up to 55 T, in temperature range 4-60 K. For studied materials, the behavior of AHE as a function of temperature was established and will be discussed. The most striking difference between AHE properties in SnMnTe and in InMnSb is different sign of AHE coefficients in the both systems. The possible explanations of this fact will be discussed.

## S4X47 **Magnetic percolation in diluted magnetic semiconductors**

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We demonstrate that the magnetic properties of diluted magnetic semiconductors are dominated by short ranged interatomic exchange interactions that have a strong directional dependence. By combining first principles calculations of interatomic exchange interactions with a classical Heisenberg model and Monte Carlo simulations, a theory that does not use any adjustable parameters is proposed, and we show that the observed critical temperatures of a broad range of diluted magnetic semiconductors, involving Mn-doped GaAs and GaN as well as Cr-doped ZnTe, are reproduced with good accuracy. We show that agreement between theory and experiment is obtained only when the magnetic atoms are randomly positioned on the Ga (or Zn) sites, whereas an ordered structure of the magnetic atoms results in critical temperatures that are much too high. This suggests that the ordering of diluted magnetic semiconductors is heavily influenced by magnetic percolation, and that the measured critical temperatures should be very sensitive to details in the sample preparation, in agreement with observations.

## S4X48 **Dielectric properties of ferroelectric - paraelectric multilayer structure**

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A simple phenomenological model allowing description of multilayer structure composed of ferroelectric and non-ferroelectric (normal dielectric) layers is proposed. The short-range interaction term describing the strength of coupling of both materials at the interlayer interfaces is introduced. The system undergoes ferroelectric phase transition at reduced temperature, depending on the ferroelectric layer thickness $d$ either as $1/d^2$ or $1/d$, and on the relation between the dielectric layer thickness $D$ and the polarization correlation length $\xi_A$. Ferroelectric instability occurs due to the softening of the lowest-frequency mode in the paraelectric phase. The electric field and polarization perpendicular to the layers result in reduction of dielectric response.

S4X49 **MICRO- AND NANO-METRIC STRUCTURE OF NIOBATE FERROELECTRIC CERAMICS PROBED WITH THERMAL AND VERY COLD NEUTRONS**

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Microstructure of niobate ceramics was studied by ultra-small angle neutron scattering (USANS), small-angle neutron scattering (SANS), and very cold neutron (VCN) spectroscopy. Ceramic samples of $(Na,Li,Sr_{0.5})NbO_3$, $(Na,Li,Cd_{0.5})NbO_3$ and $(Na,Li,Pb_{0.5})NbO_3$ systems with single-phase crystal structure were selected for study. It was shown that scattering in ceramics is mostly originated from pores. The best fit to the data was obtained for the model of polydisperse solid spheres. The pore size distribution function consists of two fractions: large pores with average size of 1 mkm and volume fraction of 1.5%, and small pores with average size of 100 $\AA$ and volume fraction is 0.2%. An average size of the large pores does not depend on the crystal structure and chemical composition of the material. These results will be helpful for solution of the accidental microstructure formation problem that blocks the development of advanced materials with controlled pore morphology.

S4X50 **Dynamics of bulk fluctuations in a lamellar phase by XPCS**

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Using the XPCS technique we measure the correlation function $g(t, q_\perp)$ of thermal fluctuations in the lamellar phase of the lyotropic system $C_{12}EO_5$/hexanol/$H_2O$, where $C_{12}EO_5$ stands for the widely studied nonionic surfactant penta-ethylene glycol mono-n-dodecyl-ether. The addition of hexanol as a cosurfactant results in a softening of the bilayers, leading to a bending constant $\kappa \sim k_B T$. As we use 200 $\mu$m thick samples, we are in the bulk regime, the effect of the solid boundaries being negligible.
The measurements were performed around the position of the first Bragg peak, at $q_z = 2\pi/d$ and for an in-plane scattering vector $q_\perp < 10^{-3}$ $\AA^{-1}$, corresponding to the undulation mode of the lamellar phase, for which the relaxation rate $\Omega(q_\perp)$ is controlled by the ratio of the bending constant $\kappa$ and the sliding viscosity $\eta_3$ and varies like $\Omega \sim q_\perp^2$.

S4X51 **New polar liquid crystalline monomers for preparation of polysiloxanes**

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Two new chiral liquid crystalline monomers with three and four chiral centres based on bilactate or trilactate units have been synthesised. The monomers have the paraelectric SmA , the ferroelectric SmC* and the antiferroelectric $SmC_A^*$ (for monomer with two lactates) phases. In polar phases, temperature dependences of spontaneous polarization, spontaneous tilt angle and complex permittivity have been measured. These monomers with polymerisable double bond at the end of the non-chiral molecular chain will be used for the preparation of liquid crystalline polysiloxanes. First polysiloxane prepared using monomer with two lactates will be presented. This work was supported by Grants: COST D14 WG15, GAČR 202/03/P011, GAČR 202/02/0840, AVOZ1-010-914.

S4X52 **Dielectric studies of new chlorinated liquid crystals**

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New chlorinated ferroelectric liquid crystals have been synthesized and investigated. Sequence of phases and phase transition temperatures have been determined from characteristic textures observed in a polarizing microscope and checked by DSC measurements. Dielectric spectroscopy was performed in a frequency range from 10 Hz to 10 MHz while changing temperature in the range of all transition temperatures. Relaxation frequencies and dielectric strengths of modes have been determined. The X-Ray study has been done to specify the order in the low temperature phase.

S4X53 **Quasiaverages and Classification Equilibrium States of Condensed Media**

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The classification of equilibrium states of condensed media with spontaneously broken symmetry is carried out. The used approach is founded on the quasiaverages concept [1]. The symmetry properties of equilibrium state are defined from requirements of the residual and spatial symmetry. This approach is founded on the representation of the residual symmetry of the degenerated equilibrium state as a subgroup of a normal phase symmetry.

The states with singlet and triplet pairing in superfluid liquid [2], the states of superfluid nuclear matter with d-pairing [3], liquid crystal states of matter are considered. Admissible conditions of the spatial symmetry and the general structure of the corresponding generator are found. For above-mentioned states the explicit form of residual symmetry generator is fined and the corresponding equilibrium structures of order parameter are obtained. The requirement of residual symmetry is expanded on the inhomogeneous equilibrium states.

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S4X54 **Rayleigh-Gans Theory Of Light Scattering In Filled Liquid Crystals**

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It is studied the dependence of light scattering on the form and dimensions of particles and the function of distribution of cylindrical particles orientation as well. Particularly, at the infinitely rigid director anchoring with particle surface the light scattering cross-section with change of light polarization exceeds essentially (by three orders of magnitude) the scattering at the weak director anchoring. The maximum of the scattering cross-section is shifted by 10-15 degrees toward the smaller scattering angles and the width of the scattering light bands increases. Besides, at the infinitely rigid director anchoring the light scattering without change of light polarization takes place but the proper light scattering cross-section is one order of magnitude smaller than at the scattering with change of light polarization.

S4X55 **The antiferroelectric liquid crystals composed of bent-shaped molecules**

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Liquid-crystalline phases formed by compounds with bent-shaped molecules have attracted particular interest of recent years. The molecules are strongly hindered from rotating due to close packing within a layer resulting in a macroscopic dipolar order. We have synthesized several non-chiral mesogens composed of bent-shaped molecules with thermally stable ester linkages and lateral methoxy substitution. All of them exhibit the antiferroelectric $B_2$ phase and some of them also a low temperature phase with an alignment within smectic layers. The phases were characterized by observation of textures in polarizing microscope, by switching properties and dielectric spectroscopy. The phase transition temperatures and values of enthalpies were determined from DSC measurements. X-ray studies performed on non-oriented samples confirmed the phase structure.

S4X56 **Soft-mode dynamics and dielectric response in SrTiO$_3$ thin films**

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The problem of reduced dielectric permittivity in thin films compared with single crystals is adressed for SrTiO$_3$ using far infrared and micro-Raman spectroscopy [1]. It is shown that the soft-mode behaviour, which is responsible for the dielectric response, is extremely sensitive to the film quality. In epitaxial films the stress from the substrate, which can easily change the phase diagram (e.g. induce ferroelectricity), plays the most decisive role. In pollycrystalline films and ceramics, grain boundaries and possible nano-cracks, treated using so called brick-wall model, can explain the observed dielectric behaviour [2].

1. T. Ostapchuk et al., Phys. Rev. B 66, 235406 (2002).
2. I. Rychetsky et al., Appl. Phys. Lett. 81, 4224 (2002).

S4X57 **Origin of Ferroelectricity in Doped Quantum Paraelectrics**

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The theory of ferroelectric (FE) phase transition in quantum paraelectrics (QP) doped by isovalent isotopic and nonisotopic impurities is presented. It is shown that the FE phase transition may occur in QP due to suppression of the zero-point atomic motion caused by the substitution of a heavy isotope for a light one. A criterion for the isotopically induced ferroelectricity is formulated. The isotope effect in SrTi($^{16}$O$_{1-x}$$^{18}$O$_x$)$_3$ discovered recently is explained. It is shown that in KTaO$_3$ the oxygen isotope exchange could not produce ferroelectric state. A nature of FE phase transition in solid solutions Sr$_{1-x}$$A_x$TiO$_3$ ($A$= Mg, Ca, Ba, Pb, Cd, Zn) and KTa$_{1-x}$Nb$_x$O$_3$ is elucidated. The off-center impurity model is checked using total energy cluster ab initio calculations. The results show that all the impurity atoms except for Mg, Zn and Li atoms move in single-well local potentials and Li in KTaO$_3$ are off-center impurities. Supported by the Russian Foundation for Basic Research (Grant N 03-02-17557).

S4X58 **New ferroelectric liquid crystals with one and two lactate groups**

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Several new liquid crystals with one, two or three chiral centres having one [A.Bubnov et al., 1999, MCLC, 328, p317] or two lactate groups have been synthesized. The materials show the BP, the cholesteric, the paraelectric SmA, the orthogonal hexatic SmB and the ferroelectric SmC* phase (the materials with the shortest alkyl chains only). Spontaneous polarization, tilt angle, helix pitch, thickness of smectic layers and an average distance between the long axes of neighbouring molecules have been measured using DSC, electro-optics, dielectric spectroscopy and X-ray techniques. The influence of the lactate groups number and the alkyl chain length on mesomorphic behaviour has been established. This work was supported by Grants: GACR 202/03/P011, GACR 202/02/0840, COST D14 WG15, No.1578 from Ministry of Sci., Tech. and Dev. Rep. of Serbia.

S4X59 **Rayleigh light scattering by large-scale inhomogeneties in filled nematics**

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Nematic liquid crystals (LCs) doped with a low concentration of small colloidal particles, now known as filled LCs, scatter light very strongly due to the defect formation in the director field around the particles. Our principal findings are that: (a) for a so-called "dipole" director configuration around the particle, the light scattering is predicted to be approximately two orders of value stronger than for a "Saturn ring" configuration; (b) incident light polarized parallel to the scattering plane gives rise to a stronger scattered angular dependence than light polarized perpendicular to it; (c) when the inclusions are cylindrical, the light scattering is relatively stronger at low scattering angles than when the inclusions are spherical; (d) for a particle network, the nature of the network domain orientational distribution influences the intensity of light scattering, but has little effect on its angular dependence.

S4X60 **Broad-band dielectric spectroscopy of relaxor ferroelectric $Sr_{0.61}Ba_{0.39}Nb_2O_6$**

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Strontium barium niobate $Sr_{0.61}Ba_{0.39}Nb_2O_6$ has an unfilled tungsten-bronze structure. Besided its ferroelectricity ($T_c \approx 350$ K), it shows pyroelectric, piezoelectric, photorefractive, non-linear and relaxor properties. Perpendicular to the polar axis its dielectric properties resemble those of a dipolar glass near and below 100 K. We present a broad-frequency-range dielectric data, from kHz to THz, collected with various techniques (IR, Raman, time domain THz spectroscopy, coaxial technique and dielectric spectroscopy) in a wide interval of temperatures (20-600 K). We confirm the presence of a strong dielectric anisotropy seen with all the experimental methods. Relaxor properties are seen in the microwave range, where a strong relaxation shifts to lower frequencies on cooling. Manifestation of this effect is seen also in the THz and FIR range. Our results are analyzed globally and relations to possible phase transitions are presented.

S4X61 **Dynamics and Green Functions of Uniaxial and Biaxial Nematic**

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Within the framework of Hamilton approach the nonlinear hydrodynamics equations for uniaxial and biaxial nematics taking into account the variation of the molecule shape are obtained. The additional hydrodynamic parameters connected with broken symmetry are introduced in terms of distortion tensor. They consist of both the anisotropy axes characterizing the orientation of molecule and parameters considering the form and conformational slackness of molecules [1]. The densities of additive integrals of motion and their flux densities are represented in terms of a thermodynamic potential. The spectra of collective excitations for nematic with disc - and rod-shape molecules are obtained. The character of an anisotropy of wave front propagation is established. It is shown that the introduction of conformation degrees of freedom reduces to a possibility of second and third sounds propagation in such nematic [2].

Dynamic equations for uniaxial and biaxial nematic in the presence of an external varying field are obtained. The hydrodynamic asymptotic of two-time Green functions for arbitrary physical quantities are found in the case with conformation degrees of freedom.

1. Ivashin A.P., Kovalevsky M.Yu., Logvinova L.V., Matskevich V.T. // Ukrainian Journal of Physics, Vol.49, N1, 2004.

2. Ivashin A.P., Kovalevsky M.Yu., Logvinova L.V. // International Journal of Quantum Chemistry, Vol. 96, 2004 (in press).

S4X62 **TWO PULSE TRANSMISSION (REFLECTION) OF LASER RADIATION BY THIN SEMICONDUCTOR FILMS**

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Peculiarities of nonlinear nonstationary transmission (reflection) of two supershort laser pulses by a thin semiconductor film, depending on amplitudes, widths, shapes of envelopes and time delays between two different incident pulses were investigated theoretically, taking into account the processes of exciton-photon interaction, excitonbiexciton conversion and twophoton biexciton excitation from ground state of the crystal. Having two incident supershort pulses, we obtain in transmission three pulses, the third of which is in the resonance with the exciton level. We established the possibility of efficient control of the transmission of one of incident pulses by change the parameters of the second pulse and predicted the effect of a strong time delay in one of transmitted pulses relative to the second. We investigated in detail and explained both the superluminal and extremely slow nonlinear light propagation phenomena.

S4X63 **Role of symmetry principles in the electromagnetically induced transparency**

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The electromagnetically induced transparency (EIT) has been observed in atoms [1] and solid media [2]. It has led to many interesting applications such as lasing without inversion [3] and light speed reduction [4]. We study the role of symmetry principles in the EIT. We show that both time-reversal symmetry and gauge symmetry guarantee that there is a destructive interference between the competing paths in an ideal three-level system. The destructive interference leads to the EIT phenomena. Thus time-reversal symmetry or gauge symmetry is at the root of EIT.

[1]J. E. Field, K. H. Hahn, and S. E. Harris, Phys. Rev. Lett. 67, 3062 (1991).
[2]B. S. Ham, P. R. Hemmer, and M. S. Shahriar, Phys. Rev. A59, R2583 (1999).
[3]A. S. Zibrov et al, Phys. Rev. Lett. 75, 1499 (1995).
[4]L. V. Hau, S. E. Harris, Z. Dutton, and C. H. Beroozi, Nature 397, 594 (1999).

S4X64    **Disorder induced e-h correlation in phototransients in semiconductors**

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In semiconductor alloys, the disorder has a twofold effect. In the individual bands, it transforms the electron and hole states into renormalized decaying polaron-like states. The disorder related statistical coupling between the bands leads on average to a kinematical $e-h$ correlation resembling the exciton phenomena. We study this for non-equilibrium transients induced by short strong optical pulses employing the non-equilibrium Green's functions obtained numerically. The effect combines a direct $e-h$ coupling and an $e-h$ mixing (light induced band hybridization), but it keeps the final state interaction character. It evolves gradually during and after the pulse: The transient polarization and the energy transfer depend on the band-band disorder correlation only at a late stage. We link, in the linear response limit, the correlation vertex with the effective Elliott factor.

S4X65    **Scintillation characteristics of Yb-doped YAlO$_3$**

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Yb-doped YAlO$_3$ single crystal scintillator (Yb-YAP) has been studied in very recent years due to its favorable features (higher density, very fast scintillation response and good mechanical and chemical stability). In this contribution the survey of luminescence and scintillation characteristics will be presented including the radiation hardness, which has not been studied yet in the literature.

S4X66    **Single-wall carbon nanotube suspension: 1.54 mkm nonlinear transmission and passive Q-switcher for self mode-locking in Er-glass laser**

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A nonlinear transmission of an aqueous suspension of single-wall carbon nanotubes (SWNT) has been investigated at wavelength 1.54 mkm. A reduction of the absorption coefficient was 3.6 cm$^{-1}$ while the initial absorption coefficient was 17 cm$^{-1}$ for the input peak laser intensity 40 MW/cm$^2$. The probe pulse duration was 250 ns. The SWNT passive Q-switcher was used for self mode-locking in Er-glass laser. The work was supported by RFBR projects 03-02-17316 and 04-02-17618.

**S4X67** **Tunable midinfrared semiconductor lasers for laser spectroscopy**

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Properties of GaSb based lasers emitting at 2.3 $\mu$m prepared by MBE were studied. The laser diodes tunable by temperature and excitation current show monomode emission with a sidemode suppression ratio of -45 dB at an operation temperature of 25 $^o$C. The threshold current of the lasers were low: 35 mA and the slope efficiency is about 0.05 W/A. The temperature dependence of the threshold current showed very good results with T0 > 110 K. The tuning rate by temperature is about 0.2 nm/K whereas the tuning rate by current is between 0.035 nm/mA and 0.05 nm/mA. The emission wavelength can by tuned by current over a range of roughly 4 nm without any mode jumps. We have compare ageing tests with noise and spectroscopic measurement prior to ageing. We have been studying how the tuning parameters of the lasers are preserved, when applied for the H.R. laser spectroscopy of methane.

**S4X68** **Phase-sensitive time-domain terahertz reflectometry**

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The time-domain terahertz (THz) spectroscopy utilizes ultrashort laser pulses and a phase-sensitive detection for investigations of complex optical constants of various materials in the far-infrared region. The THz transmission spectroscopy has become a method routinely used to this purpose but, as a drawback, it can only be used for transparent samples. With opaque samples, only the reflected THz beam can be measured; however, the need for a reference (mirror) measurement usually introduced a substantial phase error making the precise evaluation of data difficult. We review a recently developed novel method for measuring the THz reflectivity able to provide correctly both the amplitude and the phase of the THz radiation reflected from the sample. Thus it is possible to evaluate the complex optical constants of a variety of opaque materials including crystals, ceramics and thin films.

**S4Y101** **Predicting physical properties of disordered media from a single tomographic image**

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The structure of a disordered material (porous media, polymer composite) is a remarkably incoherent concept. Despite this scientists are asked to relate its properties to the "structure" of its constituent components. Integral Geometry provides a family of morphological functions $V_\nu(r, \Phi)$ for characterizing and reconstructing complex materials at porosity $\Phi$ by using parallel surfaces of distance $r$. Based on $V_\nu(r, \Phi)$ one can derive accurate expressions for percolation thresholds, transport properties and phase equilibria in porous media. We illustrate this for conductivity and elasticity of Boolean models and experimental sandstone samples. For Boolean models $V_\nu(r, \Phi)$ is uniquely determined by its value at $r = 0$ at any porosity $\Phi_0$. Thus a single image is sufficient to estimate $V_\nu(r, \Phi)$ and physical properties such as permeabilities and elastic moduli.

S4Y102 **Influence of the oxygen pressure on films properties fabricated by laser ablation from doped GGG single crystal target**

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Pulsed Laser Deposition technique is very powerful methods to fabricate complex oxide thin films because of possibility to transfer materials stoichiometry from the target to the substrate. However in our previous work we observed a strong dependence of the gallium concentration inside the film during ablation of the single $Gd_3Ga_5O_{12}$ crystal (GGG) by means of an excimer KrF laser. This nonstoichiometry could be explained by reduction of the $Ga_2O_3$ to the volatile $Ga_2O$ or by modification of ablated target, which was noticed by an EDX analyse. This phenonennon were employing to fabricate the significantly different crystalline waveguiding films doped by Pr or Yb such as GGG, $Gd_2O_3$ and $GdGaO_3$. The correlation between the oxygen pressure, spatial resolved composition of the target and composition of the film and optical properties will be presented.

S4Y103 **Connection of elastic properties for fullerene systems with intermolecular potential parameters**

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The central idea of a study involves an assumption that the intermolecular potential for fullerene system is a homogeneous function with the certain value of the homogeneity exponent. We consider fullerene molecules as spheres with high degree of symmetry interacting by inverse-power potential function. Such an approach had allowed to derive, on the grounds of similiraty, statistical valid equation of state which revealed fairly accurate results upon extrapolation of isothermal compression for fullerene in the range of thermodynamics variables where the isothermic compressibility was low. The processing of experimental data on a base of equation of state gave possibility to calculate the steepness parameter within soft sphere potential model.

S4Y104 **PHYSICO-MECHANICAL PROPERTIES OF PLASTICALLY DEFORMED CARBON STEELS**

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Magnetic, electrical, mechanical properties and parameters of the electromagnetic-acoustic transformation of patented carbon steels (0.25 and 0.7% of C) have been studied as a function of strain produced by a cold drawing with the reduction ratio of the wire cross section 0.992. Metallographic and X-ray diffraction studies show that the physical and mechanical properties are controlled by the amount and structure of cementite and ferrite, nucleation and growth of microfissures and pores, increase of microstresses etc. A correlation was found between the magnetic and mechanical characteristics of the samples. Thus by measuring the magnetic characteristics it is possible to predict the value of the mechanical parameters and to estimate the damage of a wire by the cold drawing.

S4Y105 **THE INFLUENCE OF DIVERSION FROM STOICHIOMETRY ON HEAT-CONDUCTIVITY OF ALUMINIUM-YTTRIUM GARNET.**

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The constant lattices of aluminium-yttrium garnets (AYG) which grew under high temperature from melt (T 223 K, zoned melting, stretching from melt) and under comparatively low temperature 1320 K from solution in melt are different. For example, for AYG which grew from melt a=12.0030 A, but for that grew from solution in melt 12,0063 A. The garnets got from solution in melt are more perfect on structure, but contains the greater quantity of impurities. The AYG crystals which grow from melt contains surplus of rare-earth (RE) ions but herewith contains the smaller quantity of other impurities. For these crystals it is more correct to write their chemical formula not as $Y_3Al_5O_12$, but $Y_3Al_3Y_xAl_2 - xO_12$. The value of diversion from stoichiometry according to data of different authors forms 2-3We will consider for example AYG with Lu impurity. Its chemical formula according to our writing will look as follows: $Y_3 - x_Lu_xAl_3Al_2 - y_Lu_yO_12$. Two types of defects have to influence on the reduction of heat-conductivity: 1) xLu instead of Y in c-nodes of the yttrium sublattice 2) yLu, came instead of Al in a- node. We will consider what quantity of lutetium ions substitutes aluminum in hard solution of aluminium-yttrium and aluminium lutetium garnets. For this all action of impurities on phononscattering we prescribe to influence of defect of mass. We will consider that gadolinium ions in aluminium-yttrium and aluminium lutetium garnets solution substitute only yttrium ions. The experimental data show that heat-conductivity of $Y_2.8Gd_0.2Al_5O_12$ sample aproximately complies with one of $Y_2.9Gd_0.2_Al_5O_12$ sample. In sample with x = 0.2 Lu concentration D parameter is two times greater, than at x=0.1 so and impurity of lutetium in there are distributed proportionally to distribution in sample with x= 0.1 i.e. it has $Y_2.826Lu_0.174Al_3Al_1.974Lu_0.026O_12$ composition. If analyse of heat-conductivity of "pure" AYG that is determined for it parameter of Rayleigh scattering D forms 0.025 from D parameter for sample with Lu impurity x = 0.2. If this scattering is prescribed to yttrium ions substituting Al then in approach the defect of mass a value yLu=0.012 and "pure" AYG composition has $Y_3Al_3Al_1.988Y_0.012O_12$

S4Y106 **Cross-linking of silanol-terminated PDMS with multi-functional alkoxide precursors monitored by Small Angle X-Ray Scattering.**

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In the present investigation the cross-linking of silanol-terminated poly(dimethylsiloxane), PDMS, was monitored on line by Small-Angle X-ray Scattering (SAXS), at room temperature, for at least 24 h, in 2-propanol as solvent and dibutyltin dilaurate as catalyst. When the 9-functional alkoxysilane units (PETA/AS), previously produced by Michael-addition reaction of one equivalent of pentaery-thritholtriacrylate (PETA) and three equivalents of
2-aminoethyl-3-aminopropyltrimethoxysilane (AS), was used as cross-linker agent, no scattered was observed in the experiment. When tetraethoxysilane (TEOS) was used as an additional cross-linker, the intensity of the scattering curves increased with the time. The introduction of TEOS produced ethoxi-oligomeric-silica nanoclusters, which accelerated the cross-linking reaction, giving rise to mass-fractal structures. As the cross-linking of PDMS proceeded, an increase in the mass-fractal dimension was observed, suggesting that rearrangements of the scatterers during the polycondensation reaction took place.

S4Y107 **Evaluation of crystallinity of mixed phase silicon thin films from Raman scattering spectra**

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One of the most important properties of hydrogenated microcrystalline Si thin films is crystallinity (crystallites volume fraction), which strongly influences transport and thus also the efficiency of the photovoltaic solar energy conversion, most notably by changing the open-circuit voltage. The crystallinity is usually determined from the TO phonon band of Raman spectra, decomposed into three Gaussian bands (microcrystalline, amorphous and a band associated with the bond disorder at the grain boundaries). To compare alternative ways for the decomposition, we developed a dedicated program for the nonlinear least-squares fitting of the spectra based on the Marquardt algorithm and applied it to several series of films with changing structure. We used different shapes and numbers of bands to obtain the best profile of amorphous and microcrystalline band and suggested a new way of spectra evaluation.

S4Y108 **Exploring the validity of the charged cluster model for chemical vapour deposition diamond growth**

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Diamond nucleation remains an unsolved problem. Homogeneous nucleation and the hydrogen hypothesis are generally accepted as possible mechanisms for the deposition of low-pressure diamond. Recently, the charged cluster model (CCM) was proposed as the nucleation and growth mechanism where the electric charges produced by gas activation are the heterogeneous nucleation sites for supersaturated species in the gas phase. Following the charge-induced nucleation, charged nuclei form in the gas phase but the eventual deposition of diamond or non-diamond carbon is influenced by the substrate surface. This paper explores the validity of the CCM by investigating the nucleation and growth of diamond on sapphire substrates. The effect of surface reconstruction of sapphire is also discussed within the framework of the CCM.

S4Y109 **Exact Relations between Macroscopic Moduli of Composite Media in 3 Dimensions: Application to Magnetoconductivity and Magneto-optics**

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Generic three-dimensional (3D) exact relations are found between macroscopic or bulk effective moduli of composite systems with different microstructures. These relations can be established between effective values of material coefficients of the same type (e.g. conductivity and conductivity) as well as between different types of material coefficients (e.g. conductivity and permittivity). As example of possible application of these relations, a set of Keller-like quasi-3D relations are derived for the case of columnar-shaped parallel inclusions. The microstructure in the two samples can, in general, be different. In particular, exact relations between bulk effective magnetoconductivity tensor components are found for general orientations of the applied magnetic field.

S4Y110 **CVD Synthesis and Transport Properties of Ferromagnetic Metal Filled Multiwall Carbon Nanotubes**

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In conventional semiconductor electronics the spin of the electrons is a not used quantity. However, spin dependent devices have a significant potential for data storage technology and future electronic. Due to their large spin-flip scattering length carbon nanotubes (CNTs) represent a promising candidate for spin dependent electronic devices. High magneto resistivity effects were recently discovered on ferromagnetic contacted CNTs. Ferromagnetic metal filled multiwall CNTs (MWCNTs) exhibit interesting magnetic properties. However, transport measurement results exist only on as grown two dimensional arrays of aligned Fe-filled MWCNTs. We describe the synthesis of ferromagnetic metal filled MWCNTs. We present results on single tube device transport properties at low temperatures with and without an external applied magnetic field.

S4Y111 **SMART MATERIALS AND MICROSTRUCTURAL TRANSITIONS IN COPPER BASED SHAPE MEMORY ALLOYS**

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The behavior of some materials which are often called smart materials is related to the structural changes in microscopic scale.One particular class of such materials is the shape-memory alloys which exhibit a peculiar property called shape memory effect. The origin of this phenomena lies in the fact that the material changes its internal crystalline structure with changing temperature. Metastable beta-phases of copper-based ternary alloys exhibit this peculiar property and transform from the ordered structures to the long period layered structures martensitically on cooling. Martensitic transformations in shape memory alloys occur by two lattice invariant shears in either of two opposite directions on a 110 plane of parent phase called basal plane of martensite. These planes are subjected to the hexagonal distortion with martensite formation on which atom sizes have important effect.

S4Y112 **High-Temperature Deformation Behaviour of Ti3Al-Nb Intermetallic**

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A mechanism of high-temperature plasticity has been studied in terms of stress exponent and activation energy for deformation. A ti3Al-based intermetallic was processed by hot rolling in the two-phase field to accomplish a fine grained microstructure. Compression stress-strain tests were conducted in the temperature interval 900 to 1100C and strain rates between 7x10(-5) and 2x10(-2) s(-1). Results indicate viscous-drag dislocation glide and grain boundary sliding are governing mechanisms of deformation. Activation energy for deformation suggests being dependent on solute content in the beta phase.

S4Y113 **Future material system for OEIC; GaN on Si**

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We have grown GaN on Si by using BP thin layer as a buffer crystal with growing in house made apparatus. Silicon substrate has three times heat conductivity than Al2O3 and it is electrically conductive. The quality of Si substrate is high and the price is cheap with large diameter. On the other hand, LED and LD with short wavelength are fabricated by using GaN related compound semiconductors. The crystal structure of GaN exist two types. One is wurtzite structure and the other is cubic type. The cleavage mode and the difference of electron and hole mobility are quite different. Especially, the mechanical-electric coefficient of cubic type crystal is one tenth of wurtzite structure. We have next to study the growth of BP with large diameter substrates by using mass producing machine. We have succeeded to grow BP on large size silicon substrates. It has been found the growth of GaN is strongly related to the BP morphology to fabricate devices.

S4Y114 **Dynamics of phason fluctuations in the i-AlPdMn quasicrystal**

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Using Intensity X-ray Fluctuation Spectroscopy, we measured the dynamics of phason fluctuations in the i-AlPdMn quasicrystal. From room temperature up to $500^o$C, the speckle intensity distribution displays no time evolution. At $650^o$C, the intensity correlation function decays exponentially. We find that the characteristic time decay is proportional to the square of the phason wavelength, which demonstrates that phason fluctuations are collective diffusive modes in quasicrystals.

S4Y115 **Influence of the rotational state of molecules on the electrical properties of $C_{60}$ thin films**

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The structural and electrical properties of $C_{60}$ thin films were investigated near the orientational phase transition. As the temperature is decreased, the dark and photo currents in highly crystalline pure $C_{60}$ films increase at the phase transition in a surge-like manner [E.A.Katz *et al.*, J.Appl.Phys. **93**, 3401 (2003)]. On the contrary, in $C_{60}$ films with high amorphous contents both currents decrease at the phase transition. Exposure of the samples to oxygen suppresses these critical phenomena. SPV spectroscopy studies [E.A.Katz *et al.*, J.Appl.Phys. **94**, 7173 (2003)] carried out on similar samples corroborate the conductivity results and correlate with temperature-resolved X-ray data. The proposed explanation of the effects is based on the assumption that electrical conductivity in $C_{60}$ depends strongly on the rotational state of the molecules.

S4Y116 **Flat free-standing polyelectrolyte films: Fabrication and mechanical properties**

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We have developed and applied a novel, simple and general method for measuring elastic properties of ultrathin freestanding flat films. Here, the films are polyelectrolyte multilayer films with well-controlled thicknesses between 150 and 300 nm. A film is formed using layer-by-layer self-assembly on top of an ultra-thin sacrificial pH-sensitive layer previously adsorbed to a quartz wafer. The part of the film next to the substrate is made from polyelectrolytes that allow dissolution and serves as a sacrificial layer. Upon dissolution of this layer, our polyelectrolyte film of interest is released and can be transferred to a TEM grid. The film is probed using a scanning probe microscope in force mode while being monitored in an optical microscope. Measurements can be performed both in air and under liquid.
We record the load-deformation relation, from which mechanical properties of the film are obtained. Using a continuum mechanical model, we can calculate the Youngs modulus of the multilayer. The freestanding film measurement makes it possible to determine the elastic properties for a simple, well-defined geometry without any influence of a supporting substrate. It should prove valuable for the mechanical characterization of other freestanding ultrathin membranes as well

S4Y117 **Photoinduced Magnetic Changes in Fullerene Films**

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Laser and electron beam treatment of $C_{60}$ fullerene films in the presence of oxygen leads to the appearance of ferromagnetic points. The changes in magnetic properties can be visualized by magnetooptical methods and magnetic force microscopy. Stresses in the phototransformed layer lead to the breaking of already formed polymerized patterns; therefore the topological grains appear on the film surface. The largest change of magnetic force gradient is located at the centre and at the grain boundaries. Grain boundaries are the defect regions resulting from the breaking of already formed interfullerene bonds, and they may also contain a small amount of graphite nanoparticles. As in the case of the pressure-polymerized fullerenes, the experimental data point to the defect nature of magnetic signals. Here we present a comparative study of the structural and magnetic changes in laser-exposed fullerene films depending on the irradiation conditions. Supported by the RFBR (Grant N 02-02-17617).

S4Y118 **In situ TEM straining experiments on Sigma 3 Fe-Si bicrystals**

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In situ TEM straining experiment is an important tool for investigation of plastic behaviour of materials. Invaluable information can be gained of interaction of various lattice defects during deformation. Our in situ TEM experiments were performed to study the transfer of slip bands across a coherent twin boundary.

The first in situ TEM experiments were carried out in CEA in Grenoble. The deformation stage used had two drawbacks. The maximum load was less than 12 N. However, the load necessary to induce the critical resolved shear stress for the maximum Schmid factor was often larger. A number of the prepared Fe-5.5Three orientations of the tensile axis were chosen in our experiments. In the first case, the primary slip system was common in both grains. Easy transmission of dislocations was expected according to the criteria of slip transfer [1]. However, the slip transfer was impeded by dissociation of the slip dislocations into three grain boundary dislocations [2] and no slip transfer was observed. In the other two cases, the primary slip systems were different in both grains. Two modes of deformation transfer were observed. In the first one, slip dislocations in one grain were transformed in the boundary into slip dislocations of the second grain leaving residual dislocations in the boundary. This mode is in agreement with the transfer criteria. The second mode is not predicted by the transfer criteria. The deformation by slip in one grain was transformed by the boundary into deformation twinning in the second grain.

[1] T. C. Lee, I. M. Robertson, H. K. Birnbaum, Phil. Mag. A 62 (1990) 131-153.
[2] J. Gemperlova, A. Jacques, A. Gemperle, N. Zarubova, Interface Science 10 (2002) 51-57.

S4Y119 **XPS Investigation of Ta- doped TiN thin films**

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Titanium nitride thin films containing tantalum additions were prepared by DC magnetron sputtering and annealed under vacuum at 500 °C during 1 hour. X-ray photoelectron spetroscopy (XPS) was used to investigate the chemical environment of Ta and Ti atoms in the films. Ta4f core level peak revealed the formation of Ta-N bonds whose binding energy was shifted towards higher values suggesting the presence of $TaN_xO_y$ oxinitride in addition to the formation of tantalum oxide. An additional feature was observed in the Ta4f region located between 20 and 22 eV and was more pronounced in the sample containing lower tantalum concentration. The Ti2p core level indicated that the films containing tantalum additions were more oxidized than pure titanium nitride films. Moreover, the Ti2p spectra revealed the presence of a Ti-N-O structure together with Ti-N and Ti-O bonds. The C1s signal suggests the formation of a small amount of carbides.

S4Y120 **On the Determination of the $\mu$+ site in the Magnetorefrigerant Gd5(Ge,Si)4**

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We have measured the temperature and angular dependence of the Knight shift on a spherical Gd5Ge2.35Si1.65 single crystal. The data present evidence for at least two $\mu$+ localization sites, of which the dipolar coupling tensors were extracted experimentally. Comparing the observed and calculated dipolar tensors gives no satisfactory agreement for the highly symmetrical Wyckoff sites. An exhaustive search was exploited over the lattice space. The results indicate two spacious sites which are surrounded by 4 nearest Gd atoms. This is in accordance with the known affinity of H+ to Gd. However, the discrepancy between the simulated and measured angular dependence implies a possible subtle displacement of the $\mu$+ sites when rotating about the different axes.

S4Y121 **Thermoelectric properties of heavy fermions**

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The temperature and pressure dependence of the thermoelectric power, S(T), of heavy fermion intermetallic compounds like $CeRu_2Ge_2$ are explained by the single-site Anderson model. The pressure is taken into account by changing the hybridization between the f-states and conduction band and we assume Ce $3^+$ at ambient pressure. The ground state of such a single-ion model is always a Fermi liquid but at elevated temperatures we could have a magnetic or non-magnetic fixed point, depending on the hybridization strength. The properties of the model are calculated in the non-crossing approximation, which shows that the seemingly complicated temperature dependence of S(T), and its evolution as a function of pressure, is related to the crossovers between various fixed points of the model. Different pressure dependencies of the energy scales characterizing these fixed points account for the (T,p) phase diagram of the above mentioned comounds.

S4Y122 **Electric field effect on direction of carbon nanotubes growth in CVD process**

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Carbon nanotubes (CNT) are expected to play a key role in future nanotechnology. In particular, different applications require growth CNT growth with different space orientation and assembling of the CNT with other elements such as metallic structures, conductors etc. Noncatalytical growth of multiwall carbon nanotubes oriented perpendicularly to substrate surface by CVD in DC discharge activated mixture of hydrogen and methane was demonstrated in our recent publications [1]. In this work we describe effect of variation of the external field direction near the substrate surface on direction of grown CNTs. In these experiments we use thin film metallic structures deposited onto quartz plate as substrates. The voltage applied between the elements of the planar metallic structures provides electric field with different strength and orientations. The obtained materials were examined by Raman spectroscopy, SEM and TEM to evaluate composition, structure and morphology. It was shown pronounced effect of electric field orientation on the CNT growth direction. [1] A.N. Obraztsov, A.A. Zolotukhin, A.O. Ustinov, A.P. Volkov, Yu.P. Svirko, K. Jefimovs, Diamond and Related Materials, 12 (2003) 917.

**S4Y123** **Development of vanadium-oxide resist by reactive etching in chlorine plasma**

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For development of the resist based on amorphous vanadium dioxide, a two-stage etching process has been applied [1]. First, the exposed regions of the oxide resist are developed, and then the etching of the vanadium sublayer is accomplished. In the present study, the second stage is elaborated using a plasma-etching process in chlorine. For this purpose, a cylindrical plasma reactor has been used. It was found that at low sample temperatures (below 150 $^oC$ the V-sublayer around the lines was not etched uniformly, and vanadium metal grains remained. At T = 200-250 $^oC$ the sublayer was etched out completely from the silicon substrate, and the latter was kept undamaged and smooth enough. Formation of $VCl_4$ with the melting point 153 $^oC$ seems to account for this fact, since above 200 $^oC$ that compound is volatile and is therefore removed by the vacuum system. Thus, the sample temperature has been shown to be a critical parameter for the etching of vanadium layers in Cl plasmas.

[1] A. L. Pergament, G. B. Stefanovich, E. L. Kazakova et al, Solid State Phenom., **90-91**, 97 (2003).

**S4Y124** **Commensurate Double-walled Carbon Nanotubes: Symmetry and Phonons**

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For the periodic double-walled carbon nanotubes stable configurations and full symmetry groups are found. Using this, the phonon dispersions and the displacements eigenvectors are calculated and assigned by the complete set of the conserved quantum numbers. The calculated infrared and Raman active modes match the measured values nicely. The approximate analytical frequency-diameter dependence for the breathing like, high energy and rigid layers modes is derived within perturbative model (justified by the weak inter-layer interaction). The high energy modes are scarcely influenced by the inter-layer interaction. Low temperature specific heat is below that of the ingredient single-walled) layers while the sound velocities fall close.

[1] E. Dobardzic et al., Phys. Rev. B 68 (2003) 045408
[2] M.Damnjanovic et al., Phys. Rev. B 69 (2004) 153401-1-4

**S4Y125** **Sodium, titanium orthophosphates doped with RE ions**

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Interest to the orthophosphates compounds investigation is caused by application some of this type materials for long time storage of radioactive wastes. That is why, synthesis of new compounds suitable for radioactive waste storage, investigation of their structure and its transformations under effect of temperature, atmosphere and ionizing radiation are important tasks. Crystals of sodium, titanium orthophosphates doped with rare-earth elements such as neodymium, samarium, dysprosium, and praseodymium were synthesized and investigated by spectroscopic methods at 4.2, 77, and 300 K temperatures. General luminescence characteristics were founded that allows estimating of external factors effects on structure of these materials. Therefore, the noted RE ions can be considered as luminescence probes for monitoring of state of the investigated phosphate matrices.

**S4Y126** **Structural and conductivity study of temperature-induced graphitization of amorphous fullerite C2N under pressure**

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Here we present the structural and conductivity study of samples obtained by heating of fullerite $C_{2N}$ (50< 2N < 170) from 200 up to 1000 $^oC$ at pressure 8 GPa. The electric conductivity was measured in the temperature range 4.2300 K for the samples, synthesized at temperatures from 950 to 1000 $^oC$. While at the higher temperatures (higher than 300 K) conductivity of these samples follows a typical semiconductor activation law, at lower temperatures the Mott's variable range hopping law is observed. The role of the disorder presented in the system due to the size spread of $C_{2N}$ molecules is discussed in this respect. The detailed analysis of structural and conductivity data allows us to determine the following stages of transformation in $C_{2N}$ : i) partial polymerization of fullerene molecules and increase of the polymerization degree with temperature; ii) relatively gradual destruction of fullerene molecules and formation of graphite-like clusters.

**S4Y127** **In situ diffraction study of high-pressure C60 polymerization**

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*3) Laboratoire de Cristallographie, CNRS BP166 Cedex09, 38042 Grenoble, France*
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Polymerization in pure C60 has been achieved using photochemical and high pressure-high temperature (HPHT) methods. It has been well established that, in differently synthesized polymers, the same polymeric bond, 2,2 cycloaddition, occurs. Despite this common chemical nature of both HPHT polymers and photopolymers, their crystal structures are very different. HPHT polymers display ordered structures that have been elucidated by diffraction techniques. Depending on pressure (P< 8 GPa), different polymeric phases based on 1D chains and 2D square or triangular layers are considered. In contrast, photopolymers have a disordered fcc structure, compressed with respect to the monomer, indicating a statistically random (isotropic) polymerization along all nearest neighbor directions. The origin of bond order in HPHT polymers and its absence in photopolymers, is not presently understood. Motivated by this issue, we performed an in situ HPHT diffraction study of C60 polymerization using synchrotron radiation at the E.S.R.F.. We have found that the applied anisotropic stress selects the directions of bonding inducing an anisotropic distribution of polymeric bonds. This selection is crucial to obtain ordered polymeric structures since it avoids geometrical frustration inherent to 2,2 cycloadition interfullerene bonds in the monomer fcc lattice. The photo-induced polymerization method, having no symmetry-breaking field, leads to a frustrated disordered fcc polymer.

S4Y128 **Photoelectric properties of thin-film selenium crystals with an asymetric real structure**

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*4) Ural State Technical University*

Thin-film selenium crystals with real structure asymmetry has been investigated by electron microscopy methods. In crystals with an asymmetric real structure, different crystallographic planes were parallel to the crystal surface in symmetrically equal portions of crystals as a result of rotational distortion of the lattice. This experimental fact and anisotropy of physical properties of the crystals caused, specifically, asymmetry of photoconductivity and, correspondingly, photosensitivity in symmetrically equal portions of the crystals. Asymmetry of photosensitivity values in symmetrically equal portions of a crystal should lead to different surplus concentrations of light-induced electrons and holes in these portions when the crystal is exposed to a homogeneous illumination. In turn, different concentrations of electrons and holes in symmetrically equal portions of a superconducting crystal having an asymmetric real structure should produce an electric field, which is directed perpendicular, rather than parallelly, to the light beam, unlike the electric field in the Dember effect.

S4Y129 **Synthesis, doping and adsorption properties of $TiO_2$-based nanotubes**

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Titania ($TiO_2$) has been researched throughout the chemical industry as a possible catalyst due to its powerful oxidizing properties. The catalytic performance of titania critically depends on the surface-to-volume ratio and its band gap. Here we report on the synthesis of $TiO_2$-based nanotubes which dramatically increases the active surface area. We also demonstrate the possibility of doping of $TiO_2$-NT with transition metal ions.

When a $TiO_2$-NT was exposed to $NO_2$ gas a strong adsorption of gas on the nanotube surface was observed. An echo signal was detected in pulsed EPR experiments below 200 K. A field sweep echo experiments revealed two distinct signals: three-lines at $g=2$, which are due to $NO_2$ radical, and a broad line with singularities at $g= 2.09$ and $g= 2.49$. Spin lattice relaxation time measurements demonstrated that at temperatures above 50 K the reorientation dynamics of adsorbed $NO_2$ molecules is thermally activated ($E_a= 10$ meV) while at low temperatures the molecules become nearly static on the EPR time scale. Upon extended heating at $60^oC$ in air the $NO_2$ EPR signal almost completely disappeared. The adsorption properties of $TiO_2$-NT strongly depend on the level of doping of nanotubes with transition metal ions.

S4Y130 **KEY ROLE AND THE UNIVERSALITY OF DEFORMATION MECHANISMS IN PHASE TRANSITIONS IN SOLIDS, LIQUIDS, BIOLOGICAL TISSUES (TUMOR GROWTH, AGING, ADAPTATION TO STRESS AND MEDICAL TREATMENT)**

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The work concerns with the effect of applied compressive-extension stresses (the interruptedloadings are included), S (S=0.6Sy, to 95Sy, Sy is the resolved yield stress), stress rates (10 to 1000000 MPa/s) and temperature range (T = 0.004 to 0.945Tm, Tm is the melting point) on the dislocation mean pathlengths and mean number of mobile dislocations in ionic NaCl and semiconductor InSb crystals. The important finding of the work is that the work-hardening (WH) of crystals generally varies non-monotonically to crystal softening (CS) according to the pulse length, amplitude and strain rate, the length of unloading pulse (restore time) and their total number, crystal prehistory, temperature, etc. These V-shaped frequency dependences are universal for micro- and macrodeformation, magneto- and electroplastic effects, various physical and chemical effects (impurity concentration, irradiation dose of particles, electromagnetic fields, currents, etc.) on solids, liquids, glasses, melts and biological tissues. The tumor growth,adaptation and aging are of the same nature.

S4Y131 **Quantum transport in multiwall carbon nanotubes**

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We report on magnetoresistance (MR) measurements for individual multiwall carbon nanotubes in a perpendicular magnetic field. Al backgates allowed for a considerable variation of the doping level of the tube. Gate voltage sweeps were performed for many values of the magnetic field and over a wide temperature range. At very low temperatures we observed Coulomb blockade from which we can infer the gate capacitance. After subtraction of the zero-field fluctuations, the data show clear weak localization features. Our analysis also reveals an unusual suppression of the MR at certain gate voltages, which are grouped symmetrically around the estimated position of the charge neutrality point of the tube. We attribute this to the population of subbands of the outermost nanotube shell, which is supported by band structure calculations.

S4Y132 **Disordering processes in $Cu_6P(S_{1-x}Se_x)_5Br_{1-y}I_y$ superionic conductors**

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$Cu_6PS_5X$ (X = I, Br) crystals are characterized by vacancies in copper cation sublattice. By Raman scattering and optical absorption edge studies we have separated the contribution of different types of disordering in $Cu_6P(S_{1-x}Se_x)_5Br_{1-y}I_y$ crystals: (i) Temperature-related disordering due to lattice thermal vibrations, revealed in the absorption edge smearing and phonon band broadening with temperature; (ii) Structural disordering in the crystals under investigation is of static and dynamical nature. Dynamical structural disordering is caused by hopping motion of mobile copper ions at the transition to the superionic state and increases with ionic conductivity increase; (iii) Compositional disordering in the mixed crystals due to the substitution of chalcogen and halogen anions. A multimode compositional transformation of the phonon spectra at chalcogen substitution and a one-mode transformation at halogen substitution is shown.

S4Y133 **Stability of Cu and Al crystals along displacive transformation paths**

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Stability of ground-state and higher-energy phases of Cu and Al encountered along the tetragonal (bcc-fcc), trigonal (bcc-simple cubic-fcc) and hexagonal (bcc-hcp) displacive transformation paths is studied. Total energy is computed by means of many-body semi-empirical interatomic potentials developed by Mishin and ab initio electronic structure calculations (ultra-soft pseudopotentials, VASP code). Comparison of these two calculations provides a means for the further analysis of the efficacy of the potentials. The additional testing gives further insight into the usefulness of classical potentials for atomistic modelling of lattice defects in these metals.

S4Y134 **Structure vs. temperature of $C_{60}$ intercalated with Xe**

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The $C_{60}$-Xe system was studied using the XRD technique from 7 K to room temperature. Strongly pronounced hysteresis loops have been observed in both the glass and orientational phase transition areas. The thermal expansivity is negative under cooling for $T \leq 20$ K, in agreement with earlier dilatometric data [1]. Analysis of the integrated intensities allowed us to estimate the average concentration of Xe to be $35 \pm 5$ %, in good agreement with the independent value obtained with a weighting method. The nature of the hysteresis at higher temperature is not understood. The hysteresis in the glassification region might be evidence of a new orientational-glass-like state [1].
[1] Aleksandrovskii *et al.*, Low Temp.Phys. (2004)(to be published).

S4Y135 **Growth of the multiply twinned C60 particles in the Ni+C60 composite at room temperature and ambient atmosphere**

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We report on growth of the multiply twinned C60 particles arisen in the Ni+C60 mixture at room temperature and ambient atmosphere after lengthy development. Typical 10-micrometer large C60 particles outgrow from the Ni+C60 matrix as facetted crystals with hexagonal, decahedral and icosa-hedral shapes stacking in complex manifold superstructures. The surface of the particles exhibit twinned lamella corrugations indicating the gradual nucleation and growth of the new molecular layers. It is suggested that mechanism of the particle formation is based on the phase separation of the Ni+C60 mixture which is highly stressed due to the immiscible Ni and C60 building components.

S4Y136 **Photoinduced Magnetic Changes in Fullerene Films**

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Laser and electron beam treatment of C60 fullerene films in the presence of oxygen leads to the appearance ferromagnetic points. The changes in magnetic properties can be visualized by magnetooptical methods and magnetic force miscroscopy. Stresses in the phototransformed layer lead to the breaking of already formed polymerized patterns; therefore the topological grains appear on the film surface. The largest change of magnetic force gradient is located at the centre and at the grain boundaries. Grain boundaries are the defect regions resulting from the breaking of already formed interfullerene bonds, and they may also contain a small amount of graphite nanoparticles. As in the case of the pressure-polymerized fullerenes, the experimental data point to the defect nature of magnetic signals. Here we present a comparative study of the structural and magnetic changes in laser-exposed fullerene films depending on the irradiation conditions.

S4Y137 **Photonic Microresonators Formed by Cholesteric Liquid Crystals**

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Due to the helical molecular order, cholesteric liquid crystals act as polarization-sensitive, one dimensional photonic crystals. We discuss different ways to realize cholesteric microcavities by introducing artificial defects (EPJ E 12, 553 (2003)). A conventional defect can be realized, if one interrupts the cholesteric helix by a defect layer: it acts as a cavity, sandwiched between dielectric mirrors formed by the cholesteric medium. A unique photonic defect can be realized by a twist defect, i.e. an abrupt phase jump in the cholesteric helix (V.I. Kopp, A.Z. Genack, PRL 89, 033901 (2002)). A combination of defect layer and twist defect allows for an independent tuning of resonance frequency and resonator quality. We discuss the drastic effect of a finite sample thickness on the polarization properties of the resonant modes, and compare our findings with our recent experimental results on the twist defect mode laser emission (PRL 90, 083902 (2003)).

S4Y138 **PRESSURE-INDUCED EFFECTS IN RAMAN SPECTRA OF HIPCO NANOTUBES**

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HipCO nanotubes have been studied by Raman scattering technique in diamond anvil cell. The resonant effects was observed in RBM spectral region under the pressure of 0.3 GPa. The pressure-induced RBM contour deformation was similar to that induced by a laser photon energy variation. But in our case the excitation energy was fixed. It points to changing of tube electronic structure. The gap narrowing shifts the resonance Raman conditions in favor of smaller tubes. An estimation of the gap value change (-0.06 eV at 0.3 GPa) has been based on comparison of pressure and laser photon energy influence on the RMB shape. The work is supported by NATO linkage grant, RFBR 04-02-17618.

S4Y139 **The Dielectric Response of Ordered and Disordered $Pb(Sc_{1/2}Ta_{1/2})O_3$ Thin Films**

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In this study, thin film samples prepared with a large degree of "B" site order on c-axis oriented sapphire substrates by a chemical solution deposition technique resulted in a dielectric constant maximum near 7000 at 1kHz which is similar to the reported values for bulk and single crystal specimens. However, similarly prepared disordered thin film samples displayed a dielectric constant maximum of 2000 at 1kHz, a value which is 10 times less than that observed in the bulk material. Samples with different degrees of "B" site order were prepared by controlling the temperature and time of post annealing, and were characterized by the observation of (1/2, 1/2, 1/2) superlattice reflections and dark field TEM imaging. Thin film dielectric measurements were performed "in the plane" of the film using a planar capacitor geometry.

S4Y140 **Hund's rule Magnetism in $C_{60}$ ions?**

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We investigate the occurrence of Hund's rule magnetism in $C_{60}^{n\pm}$ molecular ions, by computing the ground-state spin for all charge states $n$ from $-3$ to $+5$. The two competing interactions, electron-vibration (e-v, including Jahn Teller, favoring low spin) and electron-electron (e-e, including Hund-rule exchange, favoring high spin), are accounted for based on ab-initio coupling parameters. We calculate and classify the static Jahn-Teller distorted states for all $n$, inclusive of both e-v and e-e effects. We then correct the adiabatic result by including the zero-point energy lowering associated with softening of vibrations at the adiabatic Jahn-Teller minima. Our overall result is that while, like in previous investigations, low-spin states prevail in negative ions, Hund's rule high spin dominates all positive $C_{60}^{n+}$ ions. This suggests also that Hund-rule magnetism could arise in fullerene cation-based solid state compounds, particularly those involving $C_{60}^{2+}$.

S4Y141 **Jahn-Teller Spectral Fingerprint in Molecular Photoemission: $C_{60}$**

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The $h_u$ hole spectral intensity for $C_{60} \rightarrow C_{60}^+$ molecular photoemission is calculated at finite temperature by a parameter-free Lanczos diagonalization of the electron-vibration Hamiltonian, including the full $8\,H_g$, $6\,G_g$, and $2\,A_g$ mode couplings. The gigantic vibrational Hilbert space size called for at high temperatures is handled by means of a specially devised stochastic technique. The computed spectrum at $800\,K$ is in striking agreement with gas-phase data [1,2]. The energy separation of the first main shoulder from the main photoemission peak, $230\,meV$ in $C_{60}$, is shown to measure directly and rather generally the strength of the final-state Jahn-Teller coupling [3].

1. P. Brühwiler *et al.*, Chem. Phys. Lett. 279, 85 (1997).
2. S. E. Canton *et al.*, Phys. Rev. Lett. 89, 045502 (2002).
3. N. Manini, P. Gattari, and E. Tosatti, Phys. Rev. Lett. 91, 196402 (2003).

S4Y142 **STRUCTURAL CHARACTERIZATION OF THE PrNi$_5$ COMPOUND BY X-RAY MULTIPLE DIFFRACTION**

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The structural characterization of the magnetocaloric compound PrNi$_5$ was performed by using X-ray multiple diffraction (MD) technique. PrNi$_5$ single crystal grown by Bridgman method was analyzed with MD which occurs when a set of crystal planes (primary) parallel to the surface, is aligned to diffract the X-ray incident beam and rotated around the surface normal. Under rotation ($\phi$ axis), other planes (secondary) can also simultaneously diffract the incident beam. The plot of the primary intensity versus $\phi$, called Renninger scan (RS), shows several peaks when the relative strengths of the reflections participating in a MD process interfere constructively or dips in the converse case. Only intensity dips were measured in the PrNi5 RS since the (111) primary reflection is the strongest one and just primary to secondary energy transfer is allowed. This RS was simulated using UMWEG program [Rossmanith, J.Appl.Cryst.(2000)33,921] which allowed to obtain the lattice parameters a=4.9585(5)$\mathring{A}$ and c=3.9612(4)$\mathring{A}$ by using the adequate secondary reflections.
Support: FAPESP, CAPES and CNPq (Brazil)

S4Y143 **C60 dimerization under pressure : a combined x-ray/Raman study**

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C60 single-crystals treated at P=1-6 GPa and T=420-560 K have been studied by Raman spectroscopy and x-ray diffraction/diffuse scattering. The crystals are primarily formed of C60-C60 dimers and minor fractions of monomers, trimers, 1D and 2D polymers. They are disordered within an average cubic lattice derived from that of the monomer. The corresponding diffuse scattering intensity has been simulated by calculating the scattering produced by dimer and trimer model structures. A qualitative agreement is obtained for random positional and orientational disorder of the dimers/trimers. Possible improvements through the introduction of inter-dimer correlations are discussed.

S4Y144 **Magnetism in polymerized fullerenes**

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A room-temperature magnetically ordered state in fullerenes polymerized at certain pressure and temperature conditions has been observed in several groups. Experimental evidence exists for ferromagnetic behavior in other carbon structures: photopolymerized fullerenes, pyrolytic carbon and nanosized graphite. The explanations of the phenomena vary from intrinsic magnetism in either an ideal, or a defect-containing carbon structure to the model of magnetic proximity effects, where the presence of impurities triggers the magnetic ordering in carbon. An observation of ferromagnetic domains in large impurity-free areas of polymerized fullerenes gives a strong argument in favor of an intrinsic nature of fullerene ferromagnetism. A comparative study of fullerenes polymerized at different pressures and temperatures, as well as photopolymerized fullerenes allows us to formulate some conditions necessary for observation of magnetic ordering in fullerene solids.

**S4Y145** **Real structure analysis of nanocrystalline and submicrocrystalline materials using X-ray diffraction**

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Small-crystalline samples of metals (Cu, Fe, Mg) and semiconductors (Ge) obtained by a severe plastic deformation in UFA (Russia) were studied using conventional powder X-ray diffraction. Traditional methods of X-ray data analysis (the Williamson-Hall plot, the Warren-Averbach analysis) and new methods (the whole powder pattern fitting) and programs developed by teams of P. Scardi and T. Ungar were used. A mean grain size and a dislocation density were estimated. Their temperature dependence during an isochronal annealing was examined and results were compared with other techniques (positron annihilation, TEM). Determination of a dislocation arrangement presented a problem and an improvement of the method of analysis is desirable. A resolution of our measurements was not negligible and hence a deconvolution was necessary.

**S4Y146** **Haldane state versus magnetic order in alkali metal pyroxenes**

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We report the results of measurements of the dc magnetic susceptibility $\chi$ and of nuclear magnetic resonance (NMR) on $LiVGe_2O_6$, $NaVGe_2O_6$ and $LiVSi_2O_6$, materials with similar crystal structures in which the V ions form a quasi-one-dimensional spin $S = 1$ system; the intrachain coupling $J/k_B$ is extracted from the $\chi$ data and is established to be 47 K, 19 K and 87 K respectively. The quite large differences in the intrachain coupling are attributed to slightly different geometries of the V chains.

The NMR data suggest that the formation of the expected low-temperature Haldane phase is intercepted by an antiferromagnetic phase transition at 25 K, 18 K and 24 K respectively. This transition is attributed to a small but non-negligible interchain coupling $J_\perp/k_B$, estimated by means of a random phase approximation method, and found to be of the same order in the three compounds, namely 3.4 K, 3.4 K and 3.1 K respectively.

**S4Y147** **Determination of chiral vectors in ultra thin carbon nanotubes by multi frequency Raman spectroscopy**

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Double wall carbon nanotubes (DWCNT) were obtained by annealing entirely filled C60 peapods at 1270 C for 1 h. The Raman response of the radial breathing mode of the inner shell (RBM) of these DWCNT exhibits individual modes that originate from distinct chiralities. Utilizing different lasers as well as tuneable lasers allows for measuring the complete set of different RBM frequencies. This set of frequencies follows immediately from the geometrically possible diameters of the very narrow inner shell CNT. Can one tell which peak originates from which chirality? The best fitting assignment is found by an unbiased algorithm and shows a clear minimum.

**S4Y148** **Phase transformation investigation in Mg  rare earth based alloys by electrical resistometry**

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A high thermal stability and good mechanical properties are crucial for a wider future application of magnesium alloys. Mg alloying with rare earth elements ensures often very good hardenability due to precipitation of transient or stable phases. Relative electrical resistivity changes response on annealing conditions monitored at low reference temperature enables to identify temperature ranges of phase transformations very effectively. Electrical resistometry can be a powerful tool in the material investigation if combined with microstructure analysis in distinctive states and correlated with mechanical properties. The contribution illustrates the influence of precipitates and their dissolution on resistivity and mechanical properties of novel high performance Mg alloys during an isochronal annealing. The precipitate shape and orientation together with the thermal stability are decisive factors and determine therefore the choice of alloying element combination.

**S4Y149** **Magnetism in Polymerized Fullerenes: Theoretical Study**

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We present the results of an theoretical study of the neutral and charged fullerene dimers using ab initio Hartree-Fock and DFT methods. Calculations provide the optimized geometry, energetics and electronic structure of the neutral, charged and doubly charged fullerene dimer for the low (singlet) and high (triplet) spin states. The results suggest the possibility of high-spin ground state for the real fullerene polymers which gives us a clue to understanding carbon magnetism. Supported by the Russian Foundation for Basic Research (Grants N 02-02-17617 and 03-02-17557).

**S4Y150** **Defect state of the lattice of thin-film selenium crystals described by Riemann curvature**

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The real structure of thin-film crystals growing in amorphous films of selenium at the crystallization temperature Tcr=150-130 C was studied by the method of transmission electron microscopy. Lattices of these crystals suffer a nonuniform elastic or elastic plastic rotational distortion about two or three mutually perpendicular directions. It was shown that lattices of the studied crystals have the Riemann, rather than Euclidean, geometry. The signs of changes in the lattice geometry of the crystals were nonlinearity of bending contours in their electron microscope images and an arc-like smearing of reflections in their electron diffraction patterns. Thus, a complicated defect state of lattices of thin-film selenium crystals can be described by one parameter, namely the Riemann curvature. When the lattice geometry transforms from the Euclidean to Riemann geometry, crystallographic planes of the selenium crystal, which are initially parallel to the crystal surface, evolve to crystallographic surfaces with a non-zero Riemann curvature.

S4Y151 **Effect of Al contents and annealing on B2 FeAl studied by TMS and XRD**

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Structural changes in B2 FeAl due to variation of Al contents and annealing has been studied using transmission mossbauer spectroscopy and XRD. B2 FeAl has been prepared by reactive synthesis and. annealed in the temperature range of 573-973 K. It has been shown that the increase of Al contents results in the formation of Al antisites while Fe stoichiometric vacancies has not been observed. Most pronounced changes after annealing has been observed at the lowest and the highest Al contents. At the lowest Al contents thermally stimulated migration of Al antisites and recovery of Fe sublattice could be supposed. At the highest Al contents thermally activated Al migration from Fe sublattice may be accompanied with the formation of Fe stoichiometric vacancies.

S4Y152 **Investigation of structure of diamond C/Si heterojunction by scanning electron microscopy**

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Epitaxial structures widely used to manufacture of various electronic and optoelectronic devices. Synthetic film of diamond possesses by semiconductor and luminescent properties can be a new perspective material for electronics. The growth technology of diamond films on a cheap substrates is well advanced at present. During growth of a diamond on Si substrate at initial stage of growth formation of SiC thin buffer layer or SiC islands is possible. Whereas a sharp border between C film and Si substrate one of main requirements to structure of heterojunctions.

In the presented work the C/Si structures grown by hot-filament CVD technology was investigated by scanning electron microscopy. It is shown that C/Si structure have a sharp border between epitaxial layer and substrate and precipitates of second phase are absent.

S4Z201 **Quantum dynamics of a dimer in a periodic potential**

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An understanding of the diffusion mechanisms of atoms and molecules on surfaces is of great importance in surface science and nanotechnology. Contrary to single atoms, molecules can interact with the surface via (de-)excitations of internal vibrational modes. Furthermore, the motion onto the periodic substrate can lead to resonant excitations of these modes and to possible dissociation.

In the present study, the importance of quantum effects on the diffusion and dissociation of dimers on periodic substrates is investigated using a time-dependent wave packet method. Introducing dimensionless variables yields a rescaled Planck's constant in the resulting Hamiltonian. By varying this rescaled Planck's constant, the transition between the classical and quantum regimes is investigated.

S4Z202  **The influence of local changes of the STM resolution on the informative content of STM-images.**

I. E. Onosov[1], V. I. Visotskii[1]
*1)*

An analysis was made of the informative content of the STM-images. It was shown that the local resolution of the microscope could be taken into account to increase the informative content of the images. The possibilities of the simultaneous measurements of several surface characteristics (topographic and resolution data) were proved. The method for creating the STM-image including the topographic data and the local resolution data was suggested. These complex images have larger information capacity than usual STM-images. Thus it became possible to distinguish the surface objects which cannot be distinguished on ordinary STM-images in the constant current mode. It was concluded that the information on the local resolution could be used for the analysis of the intramolecular bonds and subatomic details of surface structures.

S4Z203  **Topographical characterization of Nitrogen bombarded Ti6Al4V with plasma ion source using AFM**

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In this work we used Atomic Force Microscopy (AFM) to study the topographical changes induced on Ti6Al4V surfaces by nitrogen ions. Nitrogen ions were introduced by a plasma ion source. The bombardment has been carried out by the energy of 30 keV at different doses between e17-e18 Ion/cm2. Experiments performed in the room temperature. Measurements of the mean surface height show that at low irradiation doses the surface inflates because of voids produced by Nitrogen bombardment. In grater doses the height decreases because of sputtering.

S4Z204  **Low-energy electron spectroscopy of GaAs**

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Low-energy (0–5 eV) electron backscattering (LEEB) technique using an original hypocycloidal electron spectrometer with high energy resolution (below 50 meV) was applied to investigate electron excitation processes of surface and bulk electron states from polished (100) and (111) surfaces of monocrystalline GaAs. Elastic and inelastic electron backscattering spectra were investigated. In LEEB spectra direct and indirect transitions of excited electrons between the density-of-states maxima in the reduced Brillouin zone can be revealed. Additionally, LEEB spectra also contain information about the excitation of surface electron states and impurity levels. These factors are responsible for the rich fine structure of the electron spectra. Our values of excitation energies for the electron states are in good agreement with the results obtained by other experimental methods as well as theoretically calculated bulk electronic energy structure of GaAs.

S4Z205 **UTILISATION OF CALORIMETRIC TUNNELING EXPERIMENTS IN CONDENSED MATTER PHYSICS**

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Calorimetric tunneling experiment (CTE) is novel experimental technique, which is based on the precise measurement of the heat generated in the vacuum-barrier tunneling junction electrodes. One utilizes the hybrid experimental configuration consisting of the low temperature STM-like tunneling setup and the semiadiabatic calorimeter for specific heat studies by means of relaxation method. Because of its origin CTE is proposed as alternative/complementary method to classical tunneling spectroscopy suitable for studies of density of states (DOS) and electron-quasiparticle interactions. Moreover, one can be used in applied research for all kind of studies, where heat generation/absorption effects accompanying the process of electron tunneling play role.

S4Z206 **Probe microscopy in using resonance tunneling**

I. E. Onosov[1], V. I. Visotskii[1]
*1)*

The possibilities of using resonance tunneling in probe microscopy are considered for improving the microscopy characteristics (including the increase in its resolution) and for realizing the fundamentally new methods of the surface investigation. The analysis is made of the features of the resonance tunneling current flowing between the tip and the sample. It is shown that in using the resonance tunneling phenomenon there is the parameter area in which the distance dependence of the current is steeper than in the ordinary (non-resonance) tunneling microscope. This fact leads to increasing the resolution at least by 1.5 times. Such increase in the resolution makes it possible to conduct more precise investigations of the dimer structure and of the intramolecular bonds between atoms and even subatomic details. The analysis is made of the possibilities of studying not only the first atomic layer of the surface but also some subsequent layers using resonance-tunneling microscopy.

S4Z207 **Surface Reconstruction Improves Free Energy of Bimetallic Nanoparticles**

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There is a growing evidence that clusters and nanoparticles have a shell periodicity and that they grow by the successive accumulation of layers. Their growth is then related to one of the oldest mathematical problems, the packing of spheres in the most dense arrangement, i.e., the perfect tetrahedral packing, which is a non filling space structure. Noncrystalline structures with fivefold axes of symmetry, such as icosahedrons and decahedrons, are composed of deformed tetrahedral units where adjacent tetrahedral faces meet at a twinning plane. Thus, the growth of noncrystalline nanoparticles and clusters can only proceed by the introduction of defects such as disclinations which lead to poly-tetrahedral structures or by close packing schemes which give well defined structures such as the Mackay icosahedron, the truncated decahedron, and the tetrahedron.

In this work we report on energetic surface reconstruction phenomenon observed on bimetallic nanoparticle systems of AuPd and AuCu, similar to a re-solidification effect observed during cooling process in lead clusters. The experimental and computational evidence that is presented shows that two of the well known defects in solid state materials that influence surface stability i. e., vacancies and surface reconstruction that tend to reduce the free energy of the systems, are present in our particles and thus these defects stabilize the structures of our bimetallic nano-systems.

S4Z208 **Thin Al films on quasicrystalline Al-Pd-Mn: The impact of structural affinities on the crystal-quasicrystal interface.**

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The vapor deposition of Al on two high-symmetry surfaces of the Al-Pd-Mn quasicrystal is monitored as a function of the substrate temperature. On the pentagonal surface, we observe five sets of Al domains with their fcc[111] axes aligned parallel to one of the five threefold-symmetry. Similar observations are made on the threefold-symmetry surface of the same alloy. An additional, yet distinctly different growth regime is found on the pentagonal surface below 250 K. These results are characteristic of the growth mode which is determined by the surface diffusion and subsequent heterogeneous nucleation of the deposited Al. On both surfaces, Al adopts the substrate symmetry by growing in fcc domains such that their orientation maximizes the coincidence of symmetry elements between the cubic and icosahedral structure. This indicates a universal geometric affinity between the periodic and the aperiodic structure.

S4Z209 **Concentration dependence of the diffusion coefficient in separating 4He-3He solid mixtures**

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The kinetics of the separation of dilute solid mixtures of $^4$He in $^3$He is investigated. A relation between the measured values of $\tau$ and the effective coefficient of mass diffusion is established using the solution of the diffusion problem with allowance for the surface resistance arising when the $^4$He impurity atoms leave the solution and enter new-phase inclusions. It is shown that an adequate description of the experimental data in the framework of the kinetic theory of tunneling transport of impurities under conditions of an appreciable interaction between them can be obtained under the assumption that the diffusion coefficient of $^4$He in $^3$He is proportional to $x^{-4/3}$. The concentration of nuclei and the average size of the region associated to each nucleus are determined. The relaxation time due to the finite resistance to the penetration of an impurity through the boundary between the matrix and new-phase inclusion is determined for the first time.

S4Z210 **SCHOTTKY AND OHMIC CONTACTS**

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In this work some aspects that determine the properties of Schottky and ohmic contacts to Si are discussed. For Schottky barrier diodes, we present results of a comprehensive study involving 10 different metals. We pay special attention to vanadium and show that its thermal and chemical stability makes it ideal for use in devices operating above room temperature and for experiments involving annealing. We discuss the effect of different metallization methods on properties of Schottky barrier diodes and show that methods which use energetic particles, such as electron beam deposition and sputter deposition, often result in inferior Schottky barrier diodes properties-the consequence of electrically active defects introduced by the energetic particles at and close to the semiconductor surface. The advantages of using V as contact material to Si are that it forms high quality, thermally stable Schottky contacts to n-Si and thermally stable ohmic contacts with low specific contact resistance to p-Si.

S4Z211 **CuPhtalocyanine-Au(110) interface formation.**

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We have performed Grazing Incidence X-Ray Diffraction (GIXRD), NEXAFS, Helium Atom Scattering (HAS) and LEED measurements at The ALOISA beamline at ELETTRA, in order to investigate the structural properties of a very thin CuPc film on Au(110), in particular the orientation of the growing layer induced by the highly anisotropic substrate. We have observed in real time the early stages of deposition by using the HAS and LEED techniques. At a supposed coverage of 1 ML, the LEED spectra reveal a (5x3) phase, as recently reported; the CuPc molecules locally induce a x3 reconstruction of the Au(110) substrate, which has been confirmed and characterized in detail by means of GIXRD rodscans. At lower coverage a very well ordered (5x5) surface structure has been observed and structurally characterized by GIXRD and NEXAFS.

S4Z212 **An Investigation of Breakdown Spots in Silicon Dioxide Film by Scanning Capacitance Microscopy**

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Scanning capacitance microscopy (SCM) has been employed to study the oxide breakdown sites on p-type Si wafer. The localized breakdown spots obviously exhibit low differential capacitance signals. In this work, the observed area of the breakdown spots approximately ranges from 6 nm to 13.5 nm in lateral direction. According to contact-mode atomic force microscopy image, the surface morphology has little effect on the SCM signal. Experimental results demonstrated that SCM is capable of detecting and investigating the localized breakdown spots of thin oxide layer. In addition, scanning capacitance spectroscopy extended from SCM also shows a great potential in providing valuable information on the oxide breakdown sites with nanometric resolution.

S4Z213 **Dipole-dependent slip at smooth solid/liquid surfaces**

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We present atomic force microscopy observations of the "effective" slippage of various non-polar and polar liquids on alkylsilane coated glass surfaces. For small contact angle non-polar liquids, the slip length decreases as one approaches a wetting transition. However, for large contact angle polar liquids it is found that the slip length is primarily influenced by the dipole moment, rather than the wettability of the liquid for the surface, where the slip length decreases with increasing dipole moment.

S4Z214 **Phase diagram of Al-Na surface alloys from first principles**

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The structural phases of $Al_xNa_{1-x}$ surface alloys have been investigated experimentally and theoretically as a function of stoichiometry ($x$) and temperature ($T$). The experimental phase diagram is reproduced on a quantitative level in *ab initio* Monte Carlo simulations, where all input parameters are obtained from density-functional theory calculations. Further, we accurately calculate the density of (configurational) states for the $Al_4Na$ surface alloy, enabling us to derive thermodynamic quantities such as free energy and entropy for the alloy. In particular, we reproduce with high precision the temperature at which an order-disorder phase transition is observed in the $Al_4Na$ surface alloy.

S4Z215 **Characterization of the metal-insulator phase transition of $Fe_{3(1-\delta)}O_4$ surfaces.**

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A sharp specific-heat peak at 123.5 K with an enormous increase of the peak-intensity in a narrow temperature step $\Delta T$ of 0.2 K was observed for the perfect stoichiometric magnetite sample ($\delta$=0), while a broad maximum around 98 K with $\Delta T$ of 20 K was found for the imperfect stoichiometric one ($\delta$=0.004). The surface Verwey transition was characterized by means of low-energy ion scattering technique using 4-8 keV $Ne^+$ and $Ar^+$ beam. The Verwey transition of these surfaces was indicated by a sharp step-rise in the temperature dependence of the scattering ion yield ($R^+(T)$) at 138 K and a wide minimum around 125 K respectively for the sample with $\delta$=0 and $\delta$=0.004. The fine structure of the $R^+(T)$ curves in the phase transition region was an indication of a complex interplay between the neutralization and re-ionization related to the interaction of ions with the surface atoms and with atoms in the deeper layers.

S4Z216 **Load dependence of atomic-scale friction on graphite: dynamical effects on the tip motion**

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Macroscopic friction is known to be proportional to the applied load. Does this behaviour still hold at the atomic scale? We study the 3D dynamics of a tip on a graphite surface at finite temperature, extracting the friction force and the corrugation of the tip-surface interaction potential as a function of the applied load. We find both friction force and potential amplitude to have a power law dependence on applied load with exponent depending on the size of the tip-surface contact. For an extended contact we can observe a dynamical locking of the tip in a commensurate state, with a corresponding increase in the friction force during the motion.

S4Z217 **Diffusion and nonlinear dynamics of adatoms and dimers on periodic surfaces**

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We study adatoms and dimers diffusing on a substrate at finite temperature T by Langevin MD. In the absence of thermal fluctuations, the dimer motion displays nonlinear features due to the interplay between the centre of mass and intramolecular motion. In particular, chaotic motion is observed for weakly bound dimers. The dimer diffusive dynamics at $T \neq 0$ does not follow Arrhenius behavior. The relation between chaotic deterministic diffusion and stochastic thermal diffusion is discussed.

S4Z218 **Microstructural and optical characterization of sol-gel derived $Al_2O_3$ thin films deposited by dip coating technique**

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$Al_2O_3$ thin films have been prepared by the sol-gel process utilizing an alkoxide of aluminum as the main precursors. The thin films were deposited onto glass substrates using dip coating technique and annealed in the temperature range 100-500 $^o$C. The microstructure of the $Al_2O_3$ thin films was studied by X-ray diffraction (XRD), and scanning electron microscopy (SEM). The as-deposited $Al_2O_3$ thin films show a homogeneous amorphous structure. The structure of the film was changed by increasing of heat treatment temperature. The optical characteristics of the films were determined using UV-Visible spectrophotometer. The aluminum oxide thin films were transparent in the visible range. The refractive index of the films depend on the heat treatment temperature.

S4Z219 **Ellipsometry study of aluminum mirrors made by diamond microgrinding in a wide spectral range**

Yaroslav V. Filipov[1], V. S. Staschuk[1], V. A. Odarich[1]

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*2)*

Most sensing to quality of a surface are ellipsometry methods that the spectral associations of optical conductivity operate with magnitudes delta and psi accordingly. Coefficient of reflection is industrially important parameter, but owing to small sensitivity is not used for the analysis at surface structure.

An examined sample is aluminum mirrors made by a method of diamond microgrinding. The working layer of metal was sputtered by a method of a vacuum ion-beam deposition or galvanic deposition in an electrolytic bath. The vacuum deposition was carried out by warming up of a material by a beam high energy electrons, and the galvanic deposition was carried out in special baths with electrolyte, which contained salt of metal, which was plotted. The different conditions of a deposition were applied by a modification of a cathode current by intermixing of an electrolyte in ultrasonic baths. Besides some samples treated during given time at a fine vacuum at specified temperatures. After drawing a layer of aluminum the chop a surface was shaped by diamond microgrinding. Optimal conditions predetermined by the technological requirements were chosen.

Ellipsometry parameters delta and psi were measured at principal angle of incidences in a wide spectral interval wavelength 0,25-17 microns (photon energy 0,07-4,96 eV). Then were calculated main optical properties: values of indexes of refraction n and absorption kapa, optical conductivity and coefficient of reflecting R.

For an evaluation of influence roughness on ellipsometrical function of a single-layer system we have taken advantage of an approximation, according to which the rough boundary of division is modeled by a gang of flat surfaces, which inclination concerning a medial line of a surface varies by a casual grade with a root-mean-square deviation alpha. The magnitude of these surfaces is considered greater, for a light wavelength.

As a result of the analysis of obtained data's for copper mirrors established correlation between quality of a surface (its roughness, thickness of an oxidized layer, thickness of an disrupted layer) and character of optical performances dependency. The concrete recommendations concerning a choice of technique and conditions of handling for deriving given parameters are submitted.

S4Z220 **Valence charge fluctuations in the ($\sqrt{3} \times \sqrt{3}$) - Pb/Si(111) system.**

Viktor Dudr[1], Natalia Tsud[2], Stanislav Fabik[3], Martin Vondráček[4], Vladimir Matolin[3], Vladimir Cháb[1], Kevin C. Prince[2]

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We have investigated the 1/3 monolayer ($\sqrt{3} \times \sqrt{3}$)-Pb/Si(111) system with core level photoemission at temperatures of 300 and 120 K. At both temperatures the Pb $5d_{5/2}$ and $5d_{3/2}$ core levels are split into two states with an intensity ratio of 2:1, as in the related Sn/Ge(111) and Sn/Si(111) systems. By doping the surface with Cs (an electron donor) or oxygen (an electron acceptor) the ratio of the intensities of the two states can be manipulated, thus identifying the states as having filled or empty dangling bonds. The results are interpreted in terms of charge fluctuations with one third of Pb atoms acting as charge donors and two thirds as acceptors. Four chemically shifted Si 2p core level peaks are found whose shifts are almost constant for the doped and undoped surfaces, with only the relative intensity changing significantly. The shifts are interpreted in the light of the charge fluctuation model (Göthelid et al, Phys. Rev. B 52, R14352 (1995)), and the integer pseudo charge model (Ballabio et al, Phys. Rev. Lett. 89, 126803 (2002)). We conclude that Pb/Si(111) fits into the pattern of group IV metals adsorbed on group IV (111) semiconductor surfaces, with Sn/Si(111) being the exceptional case, as no low temperature 3x3 structure occurs.

S4Z221 **INVESTIGATION OF PHASE TRASNFORMATIONS IN TI/SI AND CU/TIN/SI SYSTEM BY PLASMA TREATMENT**

A. Shcharbakova[1]
*1) Institute of Electronics, Belarus'*

Development of optimal conditions of plasma treatment of metal-semiconductor systems is an important problem in thin-film technology. Of particular interest is irradiation of thin-film systems with hydronitrogen plasma with the intent of formation of nitride barrier layer, e.g. TiN.
In this paper Cu/TiN/Si thin film system was obtained by Ti/Si system treatment in N-H plasma with next copper film deposition by thermal evaporation. Elements distribution along the depth in Cu/TiN/Si system was investigated by electron Auger-spectroscopy method (PHI-660 scanning Auger spectrometer).The TiN/Si interface phase composition was determined with usage electronography methods (EMR-102 electron diffractograph). Regularities of formation and growth of titanium nitride have been studied as a function of plasma irradiation parameters. Treatment of the Ti-Si system with hydronitrogen plasma makes it possible to form TiN films on silicon and results in formation of TiSi$_2$ at the interface, thus leading to changes in electrical and physical characteristics of the contact.
It was established that TiN films obtained by plasma treatment are reliable diffusion barriers for copper at temperatures up to $600^o$ C. The transition resistance measurements evidence that N-H plasma treatment lets obtain contacting barrier thin film Cu/nitride of refractory Me/Si with transition resistance $< 600$ Ohm$\mu$m$^2$.

S4Z222 **Fermi Glass Behavior of Highly Resistive Thin PbTe films**

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Typical Fermi glass behavior has been observed in nearly intrinsic PbTe films with a thickness close to the screening length (about 500 Å) deposited on mica. Earlier [1] we reported measurements of electroconductivity, Hall effect, thermopower, electric field effect (EFE), interface donor and acceptor states energy spectrum and trapping crossections. The present results on the temperature and EFE dependence of the conductivity, Hall constant and Seebeck coefficient, indicate clearly to hopping as the main mechanism of conduction. We observed a hopping conductivity for both carrier types, EFE dependence of the prefactor, a dominant contribution of the electrons to the conductivity at low temperature, a history dependent memory-like effect, and a temperature and electric field dependend relaxation of all transport coefficients.

[1] V. Sandomirsky et al, Accepted for publication in Appl. Phys. Lett. 2004; V. Sandomirsky et al, Submitted to J. of Appl. Phys. 2004

S4Z223 **Investigations of electrical proprieties of single crystalline BaTiO$_3$ by means of low-energy ion spectroscopy**

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The surface of a single-crystalline sample of BaTiO$_3$ has been investigated by low-energy ion scattering (LEIS) technique using noble gasses with the primary energy of 5-7 keV. Energy distributions of ions scattered off the surface were analyzed for an incident angle of $34^o$ and detection angle of $68^o$ and $90^o$. One very sharp peak and one broad peak were revealed attributed respectively to single ion-Ba scattering and multiply ion-surface atom scattering. Based on the LEIS results concerned to the interaction between the ionic beams with a dielectric surface and the charge state of particles the surface state dynamics have been underlined.

S4Z224 **Surface resonances in VLEED**

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VLEED (Very-Low-Energy-Electron-Diffraction) can be used to bring experimental evidence about one-dimensional sections of the electron band structure. Apart from the bulk band structure also surface resonances (specific for individual surfaces) influence the reflected electron beam intensities. Surface resonances may be related to the long-range asymptotics of the surface barrier (image states) or to the less known saturation part of this barrier (crystal induced states). Here, extreme sensitivity of the VLEED I-V curves to the saturation shape of the surface barrier will be shown and interpreted in terms of surface resonances. For demonstration and comparison with experimental data the intensities of specularly reflected electron beams from Cu(111) are computed for various saturations of the surface barrier by dynamical theory of electron diffraction.

S4Z225 **Experimental and theoretical characterization of Cu adsorption sites on a Si (111)-7x7 surface**

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Abstract Scanning tunneling microscopy (STM) experiments were used to study Cu adsorption on a Si (111)-7x7 surface as a function of applied bias voltage. The experimental results suggest that Cu atoms appear as dark spots while Si adatoms adjacent to it are imaged as gray or bright protrusions in the filled states images. The corner adatoms are observed mostly as bright spots while the 2 center adatoms appear as gray spots. Their mutual contrast is reversed in the empty state images. Based on these experimental findings, we propose that Cu is located on top of the rest atoms. In order to verify this hypothesis, we simulated theoretically STM maps by means of Density Functional Calculations (DFT) using both the Linear Combination of Atomic Orbitals (LCAO) and Plane Waves(PW) formalisms. Cu atoms were placed on top of a Si rest atom in the Si-(111)-(2x2), (4x2) and (4x4) supercells. The theoretical results agree very well with the experimental observations and suggest a charge transfer from Cu atoms to the Si adatoms. The calculated local density of states (LDOS) shows a low Cu LDOS with respect to the Si LDOS within the investigated potential range.

S4Z226 **Formation of atom wires on vicinal silicon: Ga/Si(112)-(6x1)**

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*2) Kavli Institute of NanoScience, Delft University of Technology, 2628 CJ Delft, The Netherlands*
*3) Department of Physics and Astronomy, The University of Tennessee, Knoxville, TN 37996, and Condensed Matter Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

The Ga/Si(112)-(6x1) surface consists of a self-assembled, mesoscopic array of atomic wires on a high-index Si surface [1,2]. In this work we investigate the atomic structure of this complex surface using a combination of experimental and theoretical techniques . The surface is analyzed experimentally by means of low temperature STM, STS and RBS. DFT calculations have been performed to analyze the atomic and electronic structure of more than 40 candidate structures, as well as their surface energies. STM images for these surface structures are then calculated [4] and compared with the experimental STM images.

Our results show that the Ga/Si(112)-(6x1) surface consists of two parallel rows of Ga atoms adsorbed on the terraces and at the step-edges, intersected by quasi-periodic vacancy lines. The surface is non-metallic and exhibits quasi-one dimensional character in the lowest conduction band. The passivation of the substrate's dangling bonds seems to be the main mechanism determining the structure of the overlayer.

[1] A.A. Baski, S.C. Erwin, L.J. Whitman. Surface Science 423 (1999) L265-L270.
[2] K. Yoo et al., Surface Science 514. 100-107 (2002).
[4] N. Mingo et al, Phys. Rev B 54 2225 (1996). L. Jurczyszyn et al. Surf. Sci. 482-5, 1350 (2001).

# Focused Sessions 8:30 – 10:00

*Nanoscale materials* **Room B**

F5B1 **From atomic structure of dislocations to deformation behaviour on all scales**

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The long-ranged elastic fields of dislocations mediate interactions governing many aspects of plastic deformation. However, crystal dislocations possess cores that can only be understood on the atomic level. Studies involving computer modelling are the principal source of understanding this atomic level phenomenon. We discuss first the theoretical background of such calculations, in particular the treatment of interatomic interactions. The main theme is then the demonstration of how core effects percolate to all scales. This is done by linking atomic level calculations with continuum plasticity. Using molybdenum as an example, we demonstrate that the core phenomena are reflected in deformation of both single- and poly-crystals. Finally, we show that these phenomena are common in many materials. This research was supported by the U. S. DOE and by the NSF.

F5B2 **From dislocations to strain hardening in fcc crystals: simulations and modelling**

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The characteristic stress-strain curves of FCC single crystals are modelled for the first time within a physical approach that involves no free parameter. This approach is multiscale in nature and starts at the level of the elementary mechanisms responsible for the mechanical properties of FCC crystals, the interactions and intersections and reactions of dislocations. It combines dislocation dynamics simulations, a dislocation-based constitutive model and continuum crystal plasticity code. The output is presented in the form of a set of stress-strain curves which reproduce very well the experimental data. The domain of validity of this framework and its possible extensions are discussed.

F5B3 **Diffusion and free volumes in nanoscaled materials**

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Since the pioneering work performed on nanocrystalline materials twenty years ago, diffusion in these novel types of materials has attracted permanent interest, because of the relevance of material transport for high-temperature properties. An overview will be given on recent studies of atomic diffusion in structurally stable nanocrystalline metals and alloys [1] including first measurements of self-diffusion in liquid interfaces of nanocrystalline Fe-Nd-B alloys [2]. Since diffusion is highly correlated with the presence of atomic free volumes, the results are discussed in the context with positron annihilation studies of thermal vacancy formation and interfacial free volumes.

[1] R. Würschum, S. Herth, and U. Brossmann, Adv. Engin. Mater. **5** (2003) 365

[2] S. Herth, Feng Ye, M. Eggersmann, O. Gutfleisch, and R. Würschum, Phys. Rev. Letters **92** (2004) 095901-1

*Spin polarized transport* **Room C**

F5C1 **Recent Results on Ballistic Magnetoresistance: Reproducibility, Measurements in Different Laboratorios and Electronic Effects**

Nicolas Garcia Garcia[1]

*1) Laboratorio de Fisica de Sistemas Pequenos y Nanotecnologia (CSIC) Serrano 144, Madrid 28006, Spain*

We report recent results on magnetoresistance measurement in nanocontacts that are encapsulated and stable for months. This report will inform on: 1.Reproducibility and stability of the samples as measured in different laboratories where the samples have been shipped. 2.I-V curves are nonlinear and resemble those of nanocontacts. 3.Standard stable ballistic magnetoresitance value exceeds 1000%. 4.Strong variation of the magnetoresistance with applied voltage, that implies the effect is purely electronic. 5.Temperature stability between 100 and 400K with practically constant magnetoresistance over 1000%. 6.Variation of 10% in the magnetoresistance under current injection reproducible for many cycles. 7.Time of switching smaller than 10ns within our experimental resolution. These results should open new views in spintronic for magnetic sensors.

F5C2 **Parabolic band model for magnetic tunnel junctions and related devices**

Francois Montaigne[1], Michel Hehn[1], Alain Schuhl[1]

*1) Laboratoire de Physique des Materiaux, Universit Henri Poincaré - Nancy 1*

The magnitude of the tunnel magnetoresistance is often directly linked to the spin polarisation of the density of states. This approach usually neglects the influence of the barrier. To the prejudice of the realism of the density of states, a parabolic band model can give an exact picture of the influence of the barrier on the tunnel magnetoresistance. In this framework, the Julliere model is justified for resistive enough junctions but it is shown that the polarisation depends also from the parameters of the barrier. The parabolic band model can also account for the main features of the tunnel magnetoresistance as the voltage dependence and its asymmetry, the angular dependence, the temperature dependence, the coupling and others. Characteristics of more complex devices like composite barriers, double barriers, spin filtering barrier and spin transistors can also be studied within this model. Finally, the limits of the parabolic band model will be discussed.

F5C3 **Spin injection into semiconductors through $AlO_x$, Schottky, and Zener tunnel junctions**

W. Van Roy[1], P. Van Dorpe[1], V. F. Motsnyi[1], Z. Liu[1], K. De Greve[1], G. Borghs[1], J. De Boeck[1]

*1) IMEC, Kapeldreef 75, B-3001 Leuven, Belgium*

Successful spin-injection from magnetic contacts into a semiconductor heterostructure (up to room temperature) is seen as one of the key features to realise spintronic applications. In this presentation we describe our effort in establishing spin-injection in the tunneling regime from various different ferromagnetic contacts. The device structure that is used to test the spin-injection is a III-V light emitting diode. This device has good characteristics as a detector of the injected electron spin-polarisation, in particular in combination with the oblique Hanle effect to manipulate the spins inside the semiconductor. We summarise the results on spin-injection obtained from different magnetic contact strategies: ferromagnetic metal / $AlO_x$, ferromagnetic metal / Schottky tunnel barrier and ferromagnetic semiconductor / Zener diode combination. Acknowledgements: IWT, FWO, EC Spinosa (IST-2001-33334) and Fertile (G5RD-CT-2001-00535).

### F5D1 Exchange interactions in diluted magnetic semiconductors: first-principles study

Josef Kudrnovský[1]

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The theory that combines first-principles evaluations of interatomic exchange interactions in diluted magnetic semiconductors (DMS) with a classical Heisenberg model and Monte Carlo simulations is presented. Properties of exchange interactions determined using the magnetic force theorem and the one-electron Green functions are studied in detail. The magnetic properties of DMS are dominated by short ranged interatomic exchange interactions that have a strong directional dependence. Critical temperatures of a broad range of DMS are reproduced with a good accuracy only when the magnetic atoms are randomly positioned on cation sublattices. This suggests that the ordering of DMS is influenced by magnetic percolation and that the measured critical temperatures should be very sensitive to details of the sample preparation, in agreement with experiment.
(in collaboration with V.Drchal, I.Turek, L.Bergqvist, O.Eriksson, G.Bouzerar, P.Bruno)

### F5D2 Valence and p-d exchange coupling of Mn impurities in III-V semiconductors

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*3) Oak Ridge National Laboratory, USA*
*4) MINT Center, University of Alabama, USA*

Substitutional Mn impurities in III-V semiconductors can acquire a divatlent or a trivalent configuration. For example, it is generally accepted that Mn in GaAs is in a (d5+h) configuration with five occupied d-orbitals and a delocalized hole in the valence band. In contrast, Mn in GaN and GaP is believed to be in a d4 configuration with a deep acceptor level. In order to achieve carrier-induced ferromagnetism, it is desirable that the Mn d-states couple to a shallow acceptor, which mediates the magnetic coupling. For Mn in GaAs, this is the intrinsic acceptor level introduced by the Mn impurity. For Mn in GaN and GaP, we consider the possibility of mediating exchange coupling in the d4 state via shallow acceptor levels introduced via additional impurities, such as Carbon in cubic GaN. We use the self-interaction corrected local spin density method an ab-initio electronic structure technique capable of treating localized impurity orbitals properly, to calculate the electronic structure of Mn impurities in GaN, GaP, and GaAs. In particular the method allows us to predict the p-d exchange parameters between the Mn impurity and the host valence band. For Mn in GaAs we predict p-d exchange that is in excellent agreement with experimental measurements. In GaP and GaN, we find that the Mn-d4 impurity polarizes the host valence band in a way similar to Mn-d5 in GaAs. Shallow holes that can be introduced extrinsically will be polarized anti-parallel to the Mn moments, with a p-d coupling that is larger than in GaAs due to the reduced Mn moment in the d4 state. Work supported by the Defense Advanced Research Project Agency and by the Division of Materials Science and Engineering, U.S. Department of Energy, under Contract DE-AC05-00OR22725 with UT-Battelle LLC.

F5D3 **Magneto-transport in ferromagnetic (III,Mn)V semiconductors**

Tomas Jungwirth[1]
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We review the magneto-transport properties of semiconductor structures containing ferromagnetic (Ga,Mn)As epilayers. In bulk systems, we will discuss the exprimental and theoretical understanding of the anisotropic magneto-resistance and Hall effects. In tunneling structures with one or two (Ga,Mn)As contacts we concentrate on current induced switching and tunnel magneto-resistance phenomena. All these effects demonstrate the wealth of spintronics functionalities that can be realized using ferromagnetic semiconductor materials.

*Self assembling networks: Ferrofluids, biological gels, and polymers* **Room E**

F5E1 **Structure formation in iron ferrofluids**

G.J. Vroege[1], K. Butter[1], A.P. Philipse[1]
*1) Utrecht University, Van 't Hoff Laboratory for Physical and Colloid Chemistry*

The particle structure of ferrofluids is studied in situ, by cryogenic electron microscopy, on vitrified films of iron dispersions. By means of synthesis of iron colloids with controlled particle size and different types of surfactant, dipolar particle interactions can be varied over a broad range, which significantly influences the ferrofluid particle structure. Our experiments for the first time demonstrate, in ferrofluids in zero field, a transition with increasing particle size from separate particles to linear chains of particles. Decreasing the range of steric repulsion between particles by employing a thinner surfactant layer is found to change particle structures as well. The dipolar nature of the aggregation is confirmed by alignment of existing chains and individual particles in the field direction upon vitrification of dispersions in a saturating magnetic field. Frequency-dependent susceptibility measurements indicate that particle structures in truly three-dimensional ferrofluids are qualitatively similar to those in liquid films.

F5E2 **SELF ASSEMBLING POLYMER MICROEMULSION GELS**

Gregoire Porte[1], Eric Michel[1], Jacqueline Appell[1], Jean Kieffer[1]
*1) Groupe de Dynamique des Phases Condensees, CNRS, Universite Montpellier 2*

We consider model transient networks built up from oil in water droplet microemulsions into which we add water solubles chains grafted by hydrophobic end groups. The end groups reversibly stick to the droplets so the network forms and we focus on its rheological properties. Shear thinning is observed, leading to an erratic unstable stress response at intermediate shear rates. We analyse this behaviour in terms of a very simple model which involves the reduction of the residence time of the stickers in the droplets due to the tension of the chains at high shear. The computed constitutive equation is non-monotonic with a range where the stress is a decreasing function of the rate, a feature that indeed makes homogeneous flows unstable. We discuss this instability in the light of the well documented case of giant micelles for which the non-monotonic constitutive equation results in shear banding. The notion of running liquid fracture is introduced and discussed with respect to the Bingham stress response observed in the high shear regime.

*Quasicrystal surfaces as templates for the growth of quasiperiodic systems of reduced complexity* **Room F**

### F5F1 **Pseudomorphic growth of a single element quasiperiodic ultrathin film on a quasicrystal substrate**

Ronan McGrath[1]

*1) The University of Liverpool*

Quasicrystals are metallic alloys which have unusual structural properties: they are aperiodic and display symmetries not observed in periodic materials. An ultrathin film with a periodic interlayer spacing was grown by the deposition of copper atoms on the five-fold surface of the icosahedral $Al_{70}Pd_{21}Mn_9$ quasicrystal [1]. For coverages from 5 to 25 monolayers, a distinctive quasiperiodic LEED pattern is observed. STM images show that the in-plane structure comprises rows having separations of $S = 4.5 \pm 0.2$ Å and $L = 7.3 \pm 0.3$ Å, whose ratio equals $\tau = 1.618\ldots$ within experimental error. The sequences of such row separations form segments of terms of the Fibonacci sequence, indicative of the formation of a pseudomorphic Cu film.

[1] J. Ledieu, J.T. Hoeft, D.E. Reid, J.A. Smerdon, R.D. Diehl, T.A. Lograsso, A.R. Ross and R. McGrath, Phys. Rev. Lett. 92 (2004) 135507.

### F5F2 **The effect of aperiodic symmetry on thin film growth: Xe on Al-Ni-Co**

R. D. Diehl[1]

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The structure of the 10-fold surface of decagonal Al-Ni-Co has been explored as a substrate for physisorbed gases. The clean substrate structure was characterized using low-energy electron diffraction and scanning tunneling microscopy. Adsorption isobars were peformed for Xe on this surface in the temperature range 50-80K, and the growth was found to proceed layer-by-layer for at least 3 layers. Upon adsorption of the second layer, the overlayer orders in a periodic structure, consisting of five different rotational domains of hexagonal bilayer Xe, aligned along the major symmetry directions of the quasicrystal. This adsorption system was modeled using pair potentials to describe all interatomic interactions, resulting in a very corrugated potential that enhances the effect of the Xe-Xe interaction compared to a flat surface.

### F5F3 **Single element Sb and Bi quasiperiodic monolayers on quasicrystal surfaces**

Wolfgang Theis[1]

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Single element quasicrystalline monolayers were prepared by deposition of antimony and bismuth on the fivefold surface of icosahedral $Al_{71.5}Pd_{21}Mn_{8.5}$ and the tenfold surface of decagonal $Al_{71.8}Ni_{14.8}Co_{13.4}$ [1]. Helium atom scattering and low energy electron diffraction show Bragg peaks at the bulk derived positions of the clean surfaces, revealing highly ordered quasicrystalline epitaxial films. The experimentally determined atomic density of the monolayers of $(0.8 \pm 0.3)\ 10^{15}$ cm$^{-2}$ correspond to a close packed layer with roughly one adsorbate atom per Al atom of the quasicrystalline substrate surfaces. A classification of potential atomic structure models will be presented.

[1] K. J. Franke, H. R. Sharma, W.Theis, P. Gille, Ph. Ebert and K. H. Rieder, Phys. Rev. Lett. 89, 156104 (2002)

*Hybrid biogenic and inorganic nanstructures* **Room G**

F5G1 **Semiconductor Chips with Ion Channels, Nerve Cells and Brain Tissue**

Peter Fromherz[1]

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It is a challenge to interface electrical signal processing in brains and computers on a microscopic level to get better insight of brain dynamics and to build bioelectronic devices for applications in sensorics and medicine. The nature of iono-electronic signal tranduction is elucidated by electrooptical techniques using luminescent dyes. Defined neuron-transistor junctions are assembled by combining gene technology and semiconductor technology. Silicon chips are joined to small networks grown from nerve cells of snails and given by brain tissue of rats.

Reference: P. Fromherz, Neuroelectronic Interfacing: Semiconductor Chips with Ion Channels, Nerve Cells and Brain. In: Nanoelectronics and Information Technology (Ed. Rainer Waser), Wiley-VCH, Berlin, (2003) 781-810.

F5G2 **Magnetic field manipulation of functional materials**

P.C.M. Christianen[1]

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The physical properties of organic materials, such as polymers and (self-assembled) molecular aggregates, strongly depend on their degree of orientational order. The ongoing quest for a better understanding of the intrinsic properties of novel (supra)molecular materials and improving their performance therefore requires full control over their spatial arrangement, down to the nanoscale. In this talk I will demonstrate that high magnetic fields can be used to manipulate molecular materials by utilizing the well-defined magnetic forces originating from the anisotropic diamagnetic susceptibility of the molecules. Two different examples of magnetic manipulation will be presented: 1) magnetic orientation of macromolecules and dye aggregates, leading to improved properties and 2) magnetic field induced deformation of spherical supramolecular aggregates, which enables the quantitative determination of the intermolecular forces.

*Slow light* **Room H**

F5H1 **Slow and Fast Light in Room Temperature Solids**

Robert W. Boyd[1], Matthew S. Bigelow[1], Nick N. Lepeshkin[1], Aaron Schweinsberg[1], Petros Zerom[1]
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Several methods have recently been developed to controllably slow the propagation velocity of light through material systems. These techniques offer many possibilities for applications including the development of optical delay lines, optical buffers, and optical memories, all of which can perhaps perform even at the single-photon level. Our work has involved the use of coherent population oscillations to produce a narrow spectral dip in the absorption profile of a saturable absorber. A rapid spectral variation of the refractive index accompanies this dip, leading to a large modification of the group velocity of light. Since coherent population oscillations are robust against many dephasing processes, slow light can be produced even in room-temperature solids. We have measured velocities as low as 57 m/s in a ruby crystal. In alexandrite we observe slow light propagation at certain wavelengths and superluminal (negative group velocities) propagation at others.

F5H2 **Slow light propagation in photorefractive crystals**

S. Odoulov[1], A. Shumelyuk[1], E. Podivilov[2], B. Sturman[2]
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*2) Institute of Automation and Electrometry, Russian Academy of Sciences, 630090 Novosibirsk, RUSSIA*

When recording a dynamic grating, two light waves create a highly dispersive medium where they propagate themselves. For pulse recording this leads to light deceleration or superluminal propagation. The decay time of dynamic grating (related to dielectric relaxation time) ranges from $10^{-4}$ s in semiconductors to more than $10^2$ s in wide-bandgap ferroelectric crystals. This results in narrow resonances, from 10 KHz up to few mHz and in very strong dispersion. We demonstrate experimentally the pulse propagation with $v = 0.02$ cm/s in $BaTiO_3$ and with 0.07 cm/s for gain-free pulse propagation in $Sn_2P_2S_6$. The results are in good agreement with the developed theory based on the solution of equations for slowly varying complex amplitudes of two interacting waves and time-dependent material equation.

*Quantum computing and decoherence*                                **Hall J**

F5J2      **MQT read–out of Josephson junction qubits**

Joachim Ankerhold[1], Hermann Grabert[1]
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Motivated by recent realizations of qubits with a read–out by macroscopic quantum tunneling (MQT) in a Josephson junction [1-3], we study the problem of barrier penetration in the presence of coupling to a two–state system described effectively as a spin 1/2. It is shown that whenever the diabatic potential sufaces for fixed spin intersect in the barrier region, "imaginary time" Landau-Zener transitions "under the barrier" lead to a substantial enhancement of tunneling [4]. Furthermore, ordinary, real time Landau-Zener transitions are also predicted to occur during adiabatic ramping of the qubit system towards the read-out state. Both effects lead to a loss of polarization and a corresponding loss of read-out fidelity as has been observed experimentally [5]. Tunneling out of superpositions of qubit states, that may survive due to imperfect dephasing in the detection junction, is also discussed.

[1] D. Vion et al., Science 296, 886 (2002).
[2] I. Chiorescu et al., Science 299, 1869 (2003).
[3] J.M. Martinis et al., Phys. Rev. Lett. 89, 117901 (2002).
[4] J. Ankerhold, H. Grabert, Phys. Rev. Lett. 91, 016803 (2003).
[5] D. Vion et al., in preparation.

F5J3      **analysis of decoherence of a superconducting quantum bit**

G. Ithier[1], E. Colin[1], P. Joyez[1], D. Vion[1], D. Esteve[1]
*1)*

Because they are scalable and can be addressed with electric signals, solid state devices are particularly attractive to implement quantum bits, which are the building blocks of quantum processors. On the other hand, because of strong coupling to their environment, solid state quantum bits loss quantum coherence on relatively short time scales. The Quantronium is a superconducting qubit based on small Josephson junctions, whose properties can be tuned by two external parameters, a charge and a flux. It can be manipulated by microwave resonant pulses and has an interesting working point in the external parameter space where coupling to the environment is suppressed at first order, which allows long coherence times. I will show how the coherence time can be determined using different pulse sequences, how it depends on the working point in the parameter space, and how decoherence can be reduced using spin-locking and echo techniques.

# Plenary Session 10:30 – 12:00 Hall A

P5A1 **Thermodynamic Casmir Forces**

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In electromagnetism, the Casimir force is due to the confinement of zero-point electromagnetic fluctuations between two neutral conducting plates a finite distance apart. In a completely analogous way, the confinement of critical fluctuations in an adsorbed liquid film leads to a thickness dependent correction to the free energy of the film and, therefore, a critical Casimir force between the interfaces of the film. Measurements of the thickness of of liquid He-4 and He-3-He-4 mixture films adsorbed on copper substrates confirmed the existence of the critical Casimir effect near the superfluid transition and the tricritical point transition. The force is observed to be attractive near the superfluid transition, producing a dip in the film thickness centering just below the lambda point. Near the tricritical point, the Casimir force is found to be repulsive. This work is done in collaboration with Rafael Garcia and supported by the National Science Foundation and the National Aeronautics and Space Adminstration of the United States.

P5A2 **Exploring quantum matter in optical lattice potentials**

Immanuel Bloch[1]
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At the heart of a Bose-Einstein condensate lies its description as a single giant matter wave. Such a Bose-Einstein condensate represents the most "classical" form of a matter wave, just as an optical laser emits the most classical form of an electromagnetic wave. Beneath this giant matter wave, however, the discrete atoms represent a crucial granularity, i.e. a quantization of this matter wave field, which has been inaccessible to experiments with Bose-Einstein condensates up to now. I will report on several of our most recent experiments carried out with Bose-Einstein condensates in three-dimensional optical lattices, where this matter wave quantization leads to dramatic effects in the behaviour of the many-body system. For example by controlling the potential depth of the optical lattice we are able to induce a quantum phase transition from a superfluid to a Mott insulating state, which is dominated by strong correlations between the atoms. Furthermore we show that cold collisions between the atoms lead to a periodic collapse and revival of the macroscopic matter wave field of a BEC, which cannot be explained by any of the theories for a weakly interacting Bose gas. In our most recent experiments we have been able to completely control the collisions between atoms on different lattice site. I will show how such unprecedented control can lead to highly entangled many-body states, which could be useful for quantum computation or the simulation of complex many-body Hamiltonians. Furthemore optical lattice provide a unique environment to study the physics of low dimensional quantum gases on which I will give a brief outlook.

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